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Bank Court Chambers, 2/3 Pound Way
Cowley Centre, Oxford OX4 3YF, UK

Telephone—Oxford 770125 & 772834

Telegrams—IUPAC OXFORD

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

President	—Prof. Sir HAROLD THOMPSON (UK)
Vice-President	—Dr. R. W. CAIRNS (USA)
Secretary General	—Dr. W. GALLAY (Canada)
Treasurer	—Prof. O. HORN (German Federal Republic)

IUPAC INFORMATION BULLETIN

The Bulletin provides a news medium for the various activities of IUPAC, especially of its 40 or so committees which deal with chemical topics needing regulation, standardization or codification. It includes details of forthcoming international symposia which are to be sponsored by IUPAC together with reports of such meetings which have already taken place.

Two series of Appendices to the Bulletin are issued:

- (i) Appendices on Tentative Nomenclature, Symbols, Units, and Standards
- (ii) Technical Reports

In 1973 there will be three issues of the Bulletin (Nos. 45-47). The annual subscription, inclusive of postage, will be US \$9.00 or £3.00 (surface), US \$12.00 or £4.00 (by air). Subscribers are also sent, by surface post, the two series of Appendices automatically and free-of-charge.

Irrespective of the manner in which the Bulletin is posted, the Appendices can be obtained by air at an extra cost of \$6.00 or £2.00.

Subscription orders may be placed direct, or through an agent, with the IUPAC Secretariat.

XXVII IUPAC CONFERENCE



President J. BÉNARD thanks the Lord Mayor of the City of Munich for the reception provided to IUPAC at the Town Hall



Dr. R. W. CAIRNS (on right), who became Vice-President (President-Elect) of IUPAC at the end of the Conference, talks to Prof. and Mrs. C. G. OVERBERGER (USA) during the reception at the Town Hall



Prof. Sir HAROLD THOMPSON (UK)

1973-75

XXVII IUPAC CONFERENCE

At the conclusion of the XXVII IUPAC Conference, held in Munich during the period 21-31 August 1973, Prof. Sir HAROLD THOMPSON (UK) became the President of the Union.

Curriculum Vitae of New President

HAROLD WARRIS THOMPSON was born in 1908. After attending the King Edward VII School in Sheffield, he studied at University of Oxford for his B.A. and B.Sc. He then moved to the Kaiser Wilhelm Institute for Physical Chemistry in Berlin where he obtained his Phil.D.

From 1930 he was Fellow of St. John's College at Oxford, becoming Reader in Spectroscopy at University of Oxford (1954) and Professor of Physical Chemistry (1964). His research interests have been mainly in the field of spectroscopy, especially the infrared, leading to about 290 publications alone or with coworkers in scientific journals. Since 1957 he has been Joint Editor of the international journal *Spectrochimica Acta*.

Prof. THOMPSON has a long association with IUPAC, having served as Chairman of the Commission on Molecular Structure and Spectroscopy (1955-61), Member of the Physical Chemistry Division Committee (1955-63), Bureau (1963-71), and Executive Committee (1967-71). Of particular importance has been his contribution to the evolution of the publications of the Union as Chairman of the Publications Committee (and Editorial Advisory Board) since 1957. He was elected Vice-President (President-Elect) of IUPAC in 1971. In addition, he was Chairman of the British National Committee for Chemistry during 1960-66.

He has been involved in general scientific administration at national, European, and international levels. Amongst many positions he has held, those of President of ICSU (1963-66) and Foreign Secretary of the Royal Society (1965-71) stand out. A major force in pioneering the successful series of EUCHEM Conferences, he has chaired the Organizing Committee since the start in 1964. In 1972 he became Chairman of the Great Britain-China Committee.

Among numerous honours, Prof. THOMPSON has received an Hon. D.Sc. (Newcastle, and Strasbourg), Commander of the British Empire (1959), Knight Bachelor (1968), Order of the Aztec Eagle (Mexico, 1970), Chevalier de la Legion d'Honneur (France, 1970), Grand Service Cross (German Federal Republic, 1971). His scientific honours include a Leverhulme Research Fellowship (1937), Tilden Lecturer (Chemical Society, 1943), Fellowship of Royal Society (1946), Grehm Lecturer (Zürich, 1948), Ciamician Medal (Bologna, 1959), Reilly Lecturer (Notre Dame, 1961), Cherwell Memorial Fellow (1961), Davy Medal (Royal Society, 1965), John Tate Medal (American Institute of Physics, 1966), Hon. Counsellor of Spanish Council of Scientific Research (1971), Hon. Corresponding Member of Ecuador Institute of Natural Sciences (1971).

His lifelong interest in association football stretches from being a player of no mean ability to Vice-Chairman of the English Football Association since 1967.

Other Officers

As a result of the election held at the Council meeting on 31 August, the new Vice-President (President-Elect) of the Union is:

Dr. R. W. CAIRNS (USA)

The other two Officers of the Union were elected in 1971 and continue until 1975:

Secretary General—Dr. W. GALLAY (Canada)

Treasurer —Prof. O. HORN (German Federal Republic)

Bureau

During the interval between the biennial meetings of Council, the Bureau is responsible for ensuring an orderly discharge of the functions of the Union.

In addition to the Officers of the Union, the following are automatically members of the Bureau:

Past-President—Prof. J. BÉNARD (France: 1973-5)

Division Presidents—Dr. R. N. JONES (Physical Chemistry Division: 1973-7)

Prof. V. GUTMANN (Inorganic Chemistry Division: 1973-7)

Prof. A. KJAER (Organic Chemistry Division: 1973-5)

Prof. H. BENOIT (Macromolecular Division: 1971-5)

Prof. N. TANAKA (Analytical Chemistry Division: 1973-7)

Dr. H. EGAN (Applied Chemistry Division: 1973-7)

Ex-officio—Prof. G. OURISSON (Chairman, Committee on Publications: 1973-)

Dr. D. B. TONKS (Chairman, Clinical Chemistry Section: 1971-5)

Prof. R. TRUHAUT (Chairman, Coordinating Committee for Analytical Methods for CEE and IARC: 1966-)

The 12 Elected Members of the Bureau are now:

Mr. P. M. ARNOLD (USA: 1969-77*)

Prof. Sir DEREK BARTON (UK: 1973-7)

Prof. E. D. BERGMANN (Israel: 1971-5)

Prof. A. R. H. COLE (Australia: 1973-7)

Prof. N. M. EMANUEL (USSR: 1971-5)

Prof. O. GLEMSER (German Federal Republic: 1973-7)

Prof. V. HEROUT (Czechoslovakia: 1969-77*)

Prof. O. ISLER (Switzerland: 1971-5)

Prof. S. RANGASWAMI (India: 1969-77*)

Prof. S. SHIBATA (Japan: 1967-75)

Prof. G. SMETS (Belgium: 1969-77*)

Prof. H. SUOMALAINEN (Finland: 1969-77*)

*Reelected at Munich for a further period of 4 years.

New National Adhering Organization and Associated Organizations

An application from the German Democratic Republic for membership of the Union was accepted by Council. This raises to 45 the number of member countries.

In addition, Council approved the following applications for Associated Organization status—existing international organizations whose aims and activities are in harmony with those of IUPAC:

Association of Official Analytical Chemists
International Association for Advancement of High Pressure
Science and Technology
International Association of Geochemistry and Cosmochemistry
International Committee for Rheology
International Conferences on Coordination Chemistry
International Society of Heterocyclic Chemistry

Comptes Rendus XXVII Conference

The full deliberations of Council, together with reports of meetings of nearly 50 Standing Committees, Division Committees, Sections, Commissions, and Sub-Commissions, held during the Conference in Munich, will be published early in 1974 as *Comptes Rendus XXVII Conference* (details to be announced later). The Comptes Rendus will also contain the new memberships of all these IUPAC bodies.

SCIENTIFIC COMMITTEE ON PROBLEMS OF THE ENVIRONMENT (SCOPE)

SCOPE is a standing committee of ICSU of which IUPAC is a constituent Union. It is charged on behalf of ICSU with all matters relating to the environment. IUPAC from the outset has taken a direct and deep interest in the activities of SCOPE and has a standing committee on SCOPE, as well as an official representative to SCOPE itself.

In view of the importance of chemistry in environmental matters and the substantial collaboration which has been and is being given by IUPAC to SCOPE, it is felt that an account of the aims and activities of SCOPE will be of considerable interest to the IUPAC membership and affiliates.

Early History

The XII General Assembly of ICSU, meeting in Paris on 28 September-2 October 1968, resolved that IUBS and IUGG in consultation with SCIBP should set up an *ad hoc* Committee on the Problems of the Environment, for the purpose of preparing a report upon those characteristics of the environment which man himself is altering. The report was to emphasize those problems which are of international concern, and to state whether there are those towards the solution of which the scientific competence represented by ICSU could be effectively applied.

This *ad hoc* Committee, consisting of three representatives each from IUBS and IUGG, met twice, in Washington on 1-2 March 1969 and in Stockholm on 10-11 June 1969. The second meeting of the *ad hoc* Committee was attended also by Prof. R. TRUHAUT and Prof. G. WIDMARK, who were appointed by IUPAC as Observers.

The *ad hoc* Committee in its report listed fourteen problems of significance and stated that an international nongovernmental body of scientific objectivity was required to draw up a plan and timetable of action, which would include the existing research activities in these fields. It considered that ICSU was the best available body for this task, and that the involvement of ICSU would ensure that the scientific component was of the highest quality in any advice given to government. The *ad hoc* Committee recognized that the work required close collaboration among many scientific disciplines, and the views of those in sociology, economics, and law.

The *ad hoc* Committee made two main recommendations. One was the creation of a scientific committee of ICSU with terms of reference enabling it to marshal the scientific resources of ICSU and the expertise of other disciplines in the assessment and investigation of environmental problems. The other was that ICSU promote the establishment of an International Centre for the Environment, which would include a permanent secretariat for the scientific committee and provide services for its various commissions. It recommended further that these proposed bodies cooperate fully with other groups outside of ICSU, including all relevant UN agencies, regional intergovernmental bodies, and international nongovernmental bodies.

The report of the *ad hoc* Committee, after consideration by IUBS and IUGG, was submitted to ICSU. At its X Meeting (2 October 1969) the Executive Committee of ICSU accepted the first recommendation and formally established a Special Committee, later redesignated the Scientific Committee on Problems of the Environment (SCOPE). Membership would consist of eleven (including the Chairman) to be appointed by ICSU, together

with one representative of each interested Union. The expenses involved with the latter would be the responsibility of the Union concerned.

At their meeting in Amsterdam on 16 May, 1970, the Officers of ICSU agreed to the following composition for the Committee:

ICSU	Dr. J. E. SMITH (UK) Chairman
	Prof. F. BOURLIÈRE (France)
	Dr. F. DI CASTRI (Chile)
	Dr. K. GRASSHOFF (BRD)
	Prof. T. KIRA (Japan)
	Prof. V. KOVDA (USSR)
	Prof. B. LUNDHOLM (Sweden)
	Dr. R. E. MUNN (Canada)
	Dr. K. SZESZTAY (Hungary)
	Prof. T. TASHEV (Bulgaria)
	Prof. R. TRUHAUT (France)

together with the following Union representatives:

IGU	Prof. G. F. WHITE (USA)
IUBS	Prof. D. S. FARNER (USA)
IUGG	Dr. T. F. MALONE (USA)
IUGS	Dr. J. C. FRYE (USA)
IUNS	Prof. F. J. STARE (USA)
IUPAB	Prof. M. MESELSON (USA)
IUPAC	Dr. W. GALLAY (Canada)
IUPS	Prof. J. S. WEINER (UK)

Since that time, as might be expected, the membership has changed somewhat. The present composition, listing also the Officers, is given as an Appendix.

Activities from September 1970 to September 1972

The first meeting of SCOPE was held in Madrid on 19-20 September 1970. The Committee defined its purpose and initial plan of action in the following terms: to assemble, review, and assess the information available on man-made environmental changes and the effects of these changes on man; to assess and evaluate the methodologies of measurement of environmental parameters; to provide an intelligence service on current research; and by the recruitment of the best available scientific information and constructive thinking to establish itself as a corpus of informed advice for the benefit of centres of fundamental research and of organizations and agencies operationally engaged in studies of the environment.

At this first meeting, the Committee decided on several areas of initial action and some underlying principles. Due attention would be paid to the work of existing bodies to avoid overlap as far as possible. This included the work of MAB and SCIBP. The work of SCOPE would not be composed of national programmes like IBP, but rather would fill the need for an inter-disciplinary body which would act in an advisory capacity in the whole field of the environment similar to SCOR in oceanography or SCAR in Antarctic matters. Cognizance was taken of the approaching phasing-out of IBP and the desirability of undertaking a continuation of some of its areas of interest. It was recognized that SCOPE should evolve as a body complementary in function to existing organizations and agencies. Attention would be paid also to the possible contributions which could be made to the forthcoming

UN Conference on the Human Environment at Stockholm in June 1972, although the time was very short.

It was decided that in the first instance, SCOPE would need to be rigorously selective of the problems to be investigated and to deal with a small number in depth. The criteria for selection would be the urgency of the problem, the feasibility of study, and the general applicability on a global scale, including the importance to developing countries. The problem rather than the treatment would be attacked. The Committee should have a basically advisory function, as opposed to the executive and operational. While it was visualized that eventually collaboration with social science, economics, engineering, medicine, *etc.*, would be involved, it was decided to limit initial problems to those within the competence of ICSU. In addition to man's effect on the environment, the effect of the environment on man should also be included.

The following topics were chosen at the first meeting in Madrid and assigned to working groups:

1. Global Monitoring
2. Manmodified Ecosystems: Manmade Lakes
3. Methodology for Determination of Toxic Substances in the Environment
4. International Registry of Data about Chemicals in the Environment
5. Environmental Problems in Developing Countries
6. Ecotoxicology
7. Predictive Analysis of World Ecosystems

The status of these is summarized in a later section entitled *Areas of Study*.

A second meeting of SCOPE was held in London on 14-16 January 1971. Progress in the various assigned topics by the working groups was reviewed. Particular importance had been attached to the need for representation on the Committee from Africa, India, and South-East Asia. The assent of ICSU to this proposal for three new members had been obtained and it was noted that representation from additional individual Unions would be welcomed. An analysis of the characteristics, functions, disciplinary groups, governance, funding, and methods of operation of an International Centre for the Environment was discussed by the Committee and a working party was established to consider further the objectives and functions of such a Centre and the steps needed to initiate its establishment. At this meeting, there were very active and valuable contributions made by a number of observers from UN agencies, pointing out areas where they needed assistance from SCOPE. These included UNESCO (MAB), WMO, WHO, and FAO. Interesting representations were received also from other ICSU Committees, including SCOR and SCAR, and from GARP, its joint project with WMO.

The third meeting of the Committee was held in conjunction with the First General Assembly of SCOPE in Canberra on 30 August-4 September 1971. The Committee agreed that reports should be drawn up on five additional areas of interest as follows:

1. Toxicological Evaluation of Chemical Pollutants in the Environment
2. Noise in the Human Environment
3. Problems of Urbanization
4. The Energy Crisis
5. SCIBP/SCOPE and MAB joint developments. A working group was set up to examine the ways by which the SCIBP programmes on Biomes, Processes, and Human Adaptability, could best be developed within SCOPE and in relation to MAB.

During this period in Canberra a special session was held with Mr. M. STRONG, Secretary General of the UN Conference on the Human Environment. Various aspects of the Committee's programme were discussed as well as other environmental topics. Mr. STRONG gave an account of his planning, not only for the Stockholm Conference in 1972, but for UN action in environmental problems in the years following the Conference.

The first General Assembly of SCOPE at Canberra discussed the SCOPE programme, adopted several resolutions and a Constitution of which the following is an excerpt.

Purposes and Functions

1. SCOPE is a Scientific Committee of ICSU established for the following purposes:
 - (a) To advance knowledge of the influence of man and his activities upon his environment, as well as the effects of these alterations upon man, his health, and his welfare—with particular attention to those influences and effects which are either global or shared in common by several nations.
 - (b) To serve as a nongovernmental, interdisciplinary, and international council of scientists and as a nongovernmental source of advice for the benefit of governments and intergovernmental agencies with respect to environmental problems.
2. Toward these ends, the functions of SCOPE shall include:
 - (a) Advancing studies of fundamental environmental processes, particularly those necessary to achieve a better understanding of the interactions between man and his environment.
 - (b) Devising techniques for environmental measurements with international comparability of data, and exercising scientific leadership in the design of a plan for cooperative environmental monitoring.
 - (c) Gathering, analyzing, and evaluating information concerning global and regional environmental phenomena and trends, and the effects of environment on man.
 - (d) Developing collaborative programmes among the Scientific Unions, National Members and Committees of ICSU, and other appropriate organizations including those concerned with the social sciences, in order to promote the above mentioned activities.
 - (e) Projecting current environmental trends into the future on the basis of alternative hypotheses of future human activity, population, use of natural resources, and energy requirements.
 - (f) Identifying or devising measures to minimize the adverse affects of the interaction of man and his environment.
 - (g) Acting, on behalf of ICSU, in serving as a means of communication with other organizations, such as UN agencies, on environmental questions of broader purview than those of individual Unions and Committees of ICSU.
 - (h) Promoting education in, and understanding of, environmental problems.

The fourth meeting of SCOPE was held in London on 17-18 March 1972. Progress in the activities of the various commissions and working groups was discussed. This is incorporated later in this account under the heading of areas of study. SCOPE noted reports also from working groups on the following additional topics:

1. Institutional Arrangements
2. Interactions between Environmental Transformations and Genetic and Demographic changes (MAB Project 12)
3. Model Building in Ecological Prediction
4. International Research on Human Response to Environmental Hazards
5. Special Environmental Period

Activities from September 1972 to April 1973

The Bureau of SCOPE devoted its meeting in Ottawa on 9-11 October 1972 to a review and reexamination of the course of development of SCOPE during the first two years of its existence since its first meeting in September 1970. It recognized particularly the need for a redefinition of the conceptual framework for its scientific enquiries. Certain changes in organization and structure also appeared to be indicated. Particular attention was paid to the rationale of development of its scientific programmes. In addition, stress was laid on a closer liaison with its constituent National Committees, with the individual Unions and Scientific Committees of ICSU, with other nongovernmental bodies, and with intergovernmental bodies and the programmes which they are undertaking, including the UN Environment Programme and MAB.

In this connection, Resolution 7 adopted by the XIV General Assembly of ICSU (Helsinki, 15-20 September 1972) is of particular interest and is quoted below.

"In pursuit of its principal objective of encouraging international scientific activity for the benefit of mankind,

Recognizing the need for the scientific community to respond to the issues in the present environmental situation including those considered by the United Nations Conference on the Human Environment at Stockholm June 1972, and in particular to exercise its competence in the study of the fundamental processes underlying environmental disturbances and to develop methods appropriate for all levels of study, in order to achieve a world-wide commitment and participation,

proposes to SCOPE that after making a critical identification of subjects of high priority requiring an intensive interdisciplinary effort it consider convening a series of special meetings according to the order of priority so established and that it strengthen and extend its links with disciplines not represented within ICSU including the social, engineering and medical sciences, and conservation interests. In doing so, SCOPE should use as much as possible the existing Unions and Committees of ICSU, and non-ICSU bodies, particularly of the United Nations system,

recognizes further that in achieving these objectives it will be desirable to strengthen the capacity of SCOPE to undertake this work,

urges ICSU to explore with UNESCO the creation of a SCOPE/MAB committee, and joint working groups,

invites the National Members of ICSU to explore the possibility of creating joint national committees for SCOPE and MAB and

calls upon SCOPE to define clearly those environmental problems towards which ICSU can make a distinctive contribution, for presentation to the 1973 meeting of the General Committee and to the XV General Assembly of ICSU."

The Bureau developed a statement of the broad role of SCOPE essentially in terms of biosphere processes. This conceptual framework was discussed by the Committee at its fifth meeting (Paris on 11-13 January 1973) and

agreed upon. It was considered useful to group these biosphere processes into four categories, as follows:

1. **ENERGY PROCESSES** (e.g., heat budgets of the atmosphere, land surfaces and the oceans), and the relation of energy supply and consumption
2. **BIOGEOCHEMICAL PROCESSES** (e.g., circulation, transformation, and interactions of chemical substances and particulate matter)
3. **BIOLOGICAL PROCESSES** (e.g., processes of primary and secondary production, ecosystem analysis)
4. **BIOSOCIAL PROCESSES** (e.g., human perception and environmental information, evaluation and response to manmade environmental changes)

SCOPE will emphasize the elucidation of processes which govern conditions of environmental stability and perturbation. In keeping with this, the selection of proposals for specific areas of study will be considered on the basis of criteria which reflect the aims of SCOPE and indicate the limitations of acceptability:

1. Proposals which advance knowledge of processes underlying environmental situations subject to disturbance, particularly those likely to result in irreversible change of state, or to provide data on environmental phenomena or trends of global importance.
2. Proposals which are scientifically feasible and susceptible to international interdisciplinary collaborative study.
3. Proposals which contribute to the methodology of environmental measurements with intercomparability of data.
4. Proposals contributing to the methodology of prediction of environmental trends to future time periods, and to alternative regimes of population, use of natural resources and of energy.
5. Proposals contributing scientific information on environmental problems which can aid appropriate agencies in taking action at administrative, political, or social level.

Revised Structure of SCOPE

The programme of activities will be carried out by commissions and working groups under the guidance and coordination of the Bureau. A Commission will be established for each study area, within which working groups will examine specific topics. Commissions, which are expected to be longstanding, will normally develop their activities through the following stages:

1. Review of present knowledge of the processes concerned in order to assess the available bases for management, and to identify gaps in knowledge.
2. Promotion and development of new methodology, especially of an interdisciplinary nature, to provide the new knowledge required.
3. Promotion of global research strategy and, where appropriate, of pilot projects.
4. Provision of advice and information.

It is hoped that the work of a commission will be assisted greatly by the establishment wherever possible of a centre which would act as a focal point. Such a centre might be jointly sponsored by SCOPE, the National Committee of the host country, and the host organization, under some mutually satis-

factory arrangement. The centre might be linked with a University or Research Institute at which research relevant to the aims of the Commission is in progress. Many values would accrue to all concerned in such an arrangement. It will be noted that national participation is strongly emphasized in such centres, and the interests of SCOPE lie with those problem areas where national concerns are widely shared.

It is expected that there will be interaction among commissions and working groups. The techniques of simulation modelling will be used to assist in the design of studies, the integration and assessment of present states, and the prediction of future trends.

Areas of Study

The following is a brief summary of the present status of studies which have been undertaken, and a brief description of those which have been accepted but which are as yet in the early stages of consideration.

1. *Environmental Assessment and Monitoring*

In December 1970, the Secretary General of the UN Conference on the Human Environment requested SCOPE to "prepare a report recommending the design, the parameters and technical organization needed for a coherent global environmental monitoring system making maximum use of available capabilities of existing and planned national, regional and international networks, together with such data collection and processing centres as may be required". SCOPE accepted this request. The SCOPE Commission on Monitoring drew up a report entitled *Global Environmental Monitoring*, which was issued as a SCOPE publication (SCOPE Report 1, 1971, 67 pp., \$2.00; available from SCOPE Secretariat) and presented to the UN Conference. It contained eighteen recommendations for action, and a general plan of inclusions and priorities in a global monitoring system.

This area is now being considered further by a new Commission on Environmental Assessment and Monitoring which will broaden the base of work to (a) the recognition and definition of environmental processes and problems, and to (b) the devising and refining of methods for analysis, monitoring, and assessing environmental states and trends leading to a quantitative and predictive approach suitable for future environmental planning and management.

2. *Methodology for Determination of Toxic Substances in the Environment*

A Manual of methods for the determination of selected materials that significantly alter the environment is well advanced in preparation and will be published in the near future. The analytical procedures chosen by the working group engaged in this task—virtually all experts from IUPAC—are considered to be the best and most reliable techniques having regard for the level of sensitivity required and the equipment and manpower likely to be available. In some instances, alternatives based on these criteria will be given.

The Manual will contain methods for a number of substances in various media, *i.e.*, principally air and water and also biological media in certain instances. The substances include mercury, lead, cadmium, arsenic, chromium, zinc, copper, beryllium, nickel, cobalt, vanadium, manganese, and selenium; fluoride, chloride, nitrite, nitrate, phosphate, and sulfate; oxides of nitrogen, ozone, carbon monoxide, sulfur dioxide, hydrogen sulfide, and sulfuric acid aerosol, aromatic and polycyclic hydrocarbons, and polychlorinated biphenyls and chlorinated aromatics.

3. *Manmade Lakes*

The effect of modification of ecosystems by man is of great importance and in many cases poorly understood. A study was undertaken of manmade lakes as an example of such modifications. This included the socioeconomic factors involved, the biological systems interactions and impacts, water management effects, and the methodology of examination of the gains and losses entailed in the construction of dams and reservoirs.

A report was issued under the title of *Man-Made Lakes as Modified Ecosystems* (SCOPE Report 2, 1972, 76 pp., \$2.00; available from SCOPE Secretariat).

4. *International Registry of Data about Chemicals in Environment*

The first stage of the work in this area was a feasibility study, including a pilot registry, for the establishment of a computerized compendium of data collected by national groups and UN agencies, on potentially toxic chemicals released by man into the environment. A recommendation supporting the establishment of a registry was included in the Action Plan resulting from the UN Conference on the Human Environment.

Further studies have been initiated into the detailed requirements of such a Registry. These may include data on production, use, transport pathways, molecular structure, transformations, effects on man, and other components of the biosphere and their accumulations in the biosphere.

5. *Chemical Interactions and Transformations in the Environment*

This study, which might be termed "fate of pollutants", is concerned with the physical and chemical reactions and transformations undergone by substances released by man into the environment. These reactions might be among the pollutants themselves, or between a pollutant and a naturally occurring component of the environment. The length of life of certain pollutants is of major importance in consideration of their relative importance and in monitoring considerations.

These reactions may take place in a water medium as well as in air. Changes mediated by biological agents are excluded because they will form part of the broader area of biogeochemical cycles.

A preliminary examination of this study area has been made and further studies will be conducted.

6. *Biogeochemical Cycles*

This study is related to global resources management as well as to environmental disturbance through pollutants. It includes a critical evaluation of available data on the biogeochemical cycles of carbon, oxygen, nitrogen, sulfur, phosphorus, etc., as essential dynamic components of the biosphere, with special reference to the less well known quantitative aspects of material flows through the various stages of the cycles.

Emphasis will be placed on the identification of important gaps in existing knowledge for later judgment as to priorities for action.

A preliminary evaluation of the extent of the problem has been made, and further studies will proceed.

7. *Energy and the Environment*

In this study area, a primary task will be to review environmental effects of energy use with reference to geographical, political, and socioeconomic factors, and to plan a global research strategy for investigating threshold situations in the production of waste heat in energy conversion.

A preliminary report outlining the aspects of this study area has been drawn up and further elaboration is being planned.

8. *Acoustic Environment*

The recognition of the importance of noise emissions as an agent of environmental change was recommended. A preliminary study of noise emissions as agents of environmental change recommended that the importance of noise should be recognized in environmental studies and other action. Support for this proposal was included in the Action Plan Recommendations of UN.

A contribution to the implementation of the recommendation by the UN Environment Secretariat is planned.

9. *Ecotoxicology*

This work area involves the review of available knowledge of the toxic, including sublethal, effects of various selected chemical substances on organisms and communities and hence on ecosystems. Important gaps in knowledge should be identified.

This study must involve a conceptual and methodological basis for such effects. A programme of pilot studies will be evolved, to stimulate studies in this very broad field.

10. *Ecosystem Analysis*

This will include selected studies of the processes underlying the action of a range of agents of environmental change of physical, chemical, biological, or social origin. The examination of the effects of specific pollutant substances within complex biological systems will be clearly involved within this wider framework.

Assessments of our present knowledge will be made for certain selected biomes, including tropical forests, tropical grazing lands, estuaries, and coastal areas, in order to identify gaps in knowledge, and to indicate to what extent present knowledge provides a basis for management procedures.

11. *Human Ecology*

Studies will be made of the scientific and technical issues posed by the ecological analyses of the urbanization process, including physiological, psychological, geographic, sociological, and demographic factors.

The study will include the appraisal of methodologies in relation to research design and physiological and biochemical monitoring. The most important problems will be identified.

12. *Human Response to Environmental Hazards*

This is a study of methods of examination of the ways in which human populations respond to information about manmade environmental threats, using the approaches of both natural and behavioural scientists.

This would include not only public response ranging from apathy to hysteria, but also the conditions necessary for response and subsequent action when findings are disseminated to decision-makers.

13. *Simulation Modelling*

Interdisciplinary studies in simulation modelling are planned as a contribution to the design and evaluation of studies of environmental assessment, including a wide range of variables and including the synthesis of information about present states and the prediction of likely future trends.

It is proposed also to study the methodology of impact statements which have become so important in preceding decisions on large scale human activities which involve environmental effects, e.g., dams, manmade lakes, pipelines, estuary diversions, and the like.

14. *Environmental Problems of Developing Countries*

Following a study, a report was issued on this subject which listed environmental problems, possible solutions, and the attendant difficulties in attaining these solutions.

The priorities were listed as follows: (1) degradation of ecosystems due to lack of management techniques, (2) soil destruction due to inefficient use of natural resources, (3) limitations of water resources, (4) chemical pollution, (5) urbanization and human population problems.

Consideration is now being given to the organization of a symposium on this topic.

Future Meetings

The next meeting of SCOPE in conjunction with the Second General Assembly will be held in Kiel on 4-10 October 1973.

W. GALLAY

Official Representative of IUPAC to SCOPE

Appendix

The present membership of SCOPE is as follows:

ICSU	Dr. J. E. SMITH (UK) President
	Prof. M. A. KASSAS (Egypt) Vice-President
	Dr. T. F. MALONE (USA) Secretary General
	Prof. F. BOURLIÈRE (France, SCIBP)
	Prof. F. J. FENNER (Australia)
	Prof. K. GRASSHOFF (BRD)
	Dr. R. W. J. KEAY (UK)
	Prof. T. KIRA (Japan)
	Prof. S. KRISHNASWAMY (India)
	Prof. I. KUNIN (USSR)
	Dr. B. LUNDHOLM (Sweden)
	Prof. A. MABOGUNJE (Nigeria)
	Prof. E. MEDINA (Venezuela)
	Dr. R. E. MUNN (Canada)
	Prof. O. SEOMARWOTO (Indonesia)
	Prof. T. TASHEV (Bulgaria)
UNIONS and ICSU	Prof. R. TRUHAUT (France)
	Prof. D. WASAWO (Kenya)
	Dr. H. J. BOLLE (COSPAR)
	Dr. M. PEPPER (COSPAR)
	Prof. D. S. FARNER (IUBS)
	Dr. F. N. FRENKIEL (IUTAM)
	Dr. J. W. KEELEY (IUGS)
	Dr. W. GALLAY (IUPAC)
	Prof. A. LARA (IUPAP)
	Prof. LA RIVIÈRE (IUBS)
	Prof. C. LEVINTHAL (IUPAB)
	Dr. C. LORIUS (SCAR)
	Prof. F. A. STAFLEU (ICSU)
	Prof. F. B. STRAUB (IUB)

Prof. J. S. WEINER (IUPS)
Prof. G. WHITE (IGU)
Dr. G. F. HUMPHREY (SCOR)
Dr. E. B. WORTHINGTON (COWAR)
Prof. H. YOSHIMURA (IUNS)

SECRETARIAT Executive Secretary—
Mr. H. A. W. SOUTHON
c/o Royal Society
6 Carlton House Terrace
London SW1Y 5AG, UK

REFERENCE MATERIALS FOR TRACE ANALYSIS BY RADIOCHEMICAL METHODS

Under its current project on 'Reference Materials' and at the request of one of its Members, the IUPAC Commission on Analytical Radiochemistry and Nuclear Materials has examined the data available on some materials produced by the US National Bureau of Standards (NBS) with a view to their suitability for use as standard reference materials for radioanalytical methods of analysis.

The Commission is now in a position to recommend the use of three of these materials as appropriate for this kind of method. The materials are recommended for calibration of radioanalytical methods only in the case of those trace elements which have been officially certified by NBS, but the homogeneity tests to which they have been submitted indicate that they are also probably suitable for interlaboratory comparisons on other elements.

The Commission wishes also to encourage further radioanalytical studies of these materials by other laboratories to improve their applicability, considering that they are available in relatively large amounts and that the work done to prepare them covers the greatest part of the effort and expense necessary to fill the acute need of this type of material in the radioanalytical community.

Materials Recommended

1. *Dried Orchard Leaves*. Recommended for use as a reference material for trace determination by radioanalytical methods in botanical and other biological samples. It is currently certified by NBS for the content of 14 elements (Fe, Mn, Na, Pb, B, Zn, As, Cu, Rb, Ni, Hg, Cd, Se, U, which range from some tens to some hundredths ppm) and information data are available on about 12 more elements.
2. *Doped Glass Wafers, Nominal Trace Concentration 1 ppm*. Recommended for use as a reference material for trace determination by radioanalytical methods in samples of geological origin. It is currently certified for 8 elements (Cu, Pb, K, Rb, Ag, Sr, Th, U) and information data are available on about 14 more elements.
3. *Doped Glass Wafers, Nominal Trace Concentration 0.02 ppm*. Recommended for the same use as the previous material. It is currently certified for 5 elements (Pb, K, Sr, Th, U) and information data are available on about 12 more elements.

M. B. A. CRESPI

REPORTS OF IUPAC BODIES

COMMISSION ON TEACHING IN CLINICAL CHEMISTRY

Copenhagen, 17 June 1972

Present: Prof. M. RUBIN (Chairman), Prof. P. LOUS, Prof. A. L. LATNER, Dr. M. ROTH (Titular Members); Prof. A. DEFALQUE (Associate Member).

A review was carried out of the draft Monograph on teaching of clinical chemistry. It was decided that Section 1.1, referring to the background of the subject (pp. 1-6), required some editing to be more concise.

In Section 2, the *Introduction* required greater definition in terms of the scope and nature of clinical chemistry as a subject area. It was agreed that modification of the present text along the lines of the 'Zuckerman Report' (UK) was indicated.

In Section 3, *History* was considered too anglicized in its present form with some significant omissions of historic contributions to the subject from countries such as Germany, etc.

3.1. Addition of the development of the subject from the viewpoint of the evolution of ideas and the growth of the size of laboratories, increased role of chemical science in the medical arts, increased variety of tests, and the role of increasing quality control appeared to be indicated.

3.1.3. The need to extend the historic development of speciality journals in clinical chemistry was considered significant.

3.2.1. *Present Status:* the addition of a treatment of the application of clinical chemistry to preventive health was accepted.

3.2.2. The Commission reviewed the reports of the subcommittees which had separately completed their assignments in dealing with the 'physicians viewpoint as to the required education in medical subjects required by the nonphysician chemist' and 'the required education in chemical and physical science for physicians in clinical chemistry'. Both reports were considered pertinent and significant for inclusion in this Section.

3.2.3. Some suggestions were made for this section dealing with the role of basic research education for eliciting underlying biochemical mechanisms of disease.

3.4. The section dealing with the legal controls of chemists working in this field was considered to require some elaboration.

Considerable time was expended on the problem of the format uniformity of the many national reports on teaching of clinical chemistry now in hand. Because of the communication problem the Commission decided to undertake the redrafting of these reports if rapid response from the respective countries could not be obtained. The major problem of setting a cutoff point of the status of the subject in a given country had extensive debate. It was pointed out that the subject of clinical chemistry was in a state of great flux. Changes in legislation and teaching programmes were occurring frequently. The Commission decided that the urgency of international guidelines on the subject dictated against further delay in the present report.

M. RUBIN

COORDINATING COMMITTEE FOR ANALYTICAL METHODS FOR CEE AND IARC

Paris, 10 April 1973

Present: Prof. R. TRUHAUT (Chairman), Prof. F. PELLERIN (Secretary),
Dr. H. EGAN, Dr. R. MARCUSE.

Minutes of Meeting at Kungälv, Göteborg*

1. The methods fulfilling the Contract for 1972 had been sent to CEE on 30 October 1972 (1227/RR/CAD/72). To date no comments had been received from CEE.
2. There was an error in the text of method 31/72 RE 1 sent to CEE. 'Free acid in salicylate esters and sodium salicylate' should read 'Free acid in ethyl and n-propyl esters of *p*-hydroxybenzoates'.
3. The following method could be sent to CEE: Limit Test for Salicylic Acid in the Ethyl and n-Propyl Esters of *p*-Hydroxybenzoic Acid and their Sodium Derivatives. This method had been prepared by Prof. PELLERIN on the basis of method 31/68.
4. Method 11/68 RE 1 (Determination of Mercury in Food Additives) was circulated within IUPAC on 24 November 1972 (1386/RR/CAD/72) for consideration for the 1973 Contract.

Relations between IUPAC and CEE

The Scientific Commission of CEE had not met for more than 6 months; because of this no comments had been given and a joint IUPAC-CEE meeting discussed at Kungälv had not been organized. Prof. TRUHAUT proposed to go to Brussels to discuss with Mr. L. G. RABOT (Director General of Agriculture) and Mr. I. GAERNER (Secretary of the Scientific Commission) the scientific, financial (increase of payment by CEE), and economic problems relating to IUPAC-CEE Contracts. Prof. TRUHAUT's journey was subject to the approval of the Officers of IUPAC and Dr. EGAN would contact the IUPAC Secretariat about this matter.

On the subject of reports for CEE, Dr. MARCUSE underlined the problem of standardization. This problem would arise in various matters during this meeting.

Preparation of Methods for 1973 Contract

The choice of some methods for the 1973 Contract was made in Kungälv/Göteborg last year, taking into account the fact that CEE would like the programme concerning antioxidants and other food additives to be finalized in 1973. Dr. EGAN had asked various Members of the Food Section and Commission on Analytical Reactions and Reagents to propose methods. The Coordinating Committee then discussed the methods proposed.

1. Trace Metals in Food Colours by X-ray Fluorescence (replaced method 16/68). The method proposed by Dr. P. W. WATLINGTON would be circulated.
2. Limit Test for Selenium. This method was sent to CEE in October 1972 (27/72 RE 1).

*See *Inf. Bull.* No. 44 (December 1972), p. 59.

3. Uranium in Food Colours. The problem of detection was resolved with method 1 above.
4. Polycyclic Aromatics in Water Soluble Colours. Information would be requested from Dr. E. O. HAENNI.
5. Fatty Acids in Sodium, Potassium, and Calcium Lactates. The method presented by Sté Mallinckrodt would be edited by Dr. EGAN for circulation.
6. Polycyclic Acids in Benzoic Acid and its Sodium, Potassium, and Calcium Salts. This required the use of gas chromatography coupled with mass spectrometry. It would be the subject of further study by IUPAC. Mention should be made in the general introduction that the application of methods of this type required relatively specialized apparatus. In this case it would perhaps be more reasonable to give only general directions.
7. α -Naphthol in Sodium *o*-Phenylphenate. The method proposed by Dr. P. L. SCHULLER would be circulated.
8. Aromatic Amines in Diphenyl. The method proposed by Prof. PELLERIN would be circulated.
9. Benzene in Diphenyl
10. Organically-bound Chlorine in Benzoic Acid and Sodium, Potassium, and Calcium Benzoates. The method proposed by Dr. SCHULLER would be circulated.
11. Phenolic Derivatives in Diphenyl. Information would be sought from CEE on the necessity to introduce such criteria, no basis for which could be found in the scientific literature. Meanwhile, an experimental study would be made by Prof. PELLERIN.
12. Diphenyl Ether in Sodium *o*-Phenylphenate. Information would be sought from CEE on the necessity for such purity criteria.
13. Water Content of Sodium Nitrate. The method proposed by Dr. SCHULLER would be circulated.
14. Nitrites in Sodium and Potassium Nitrates. The method proposed by Dr. SCHULLER would be circulated.
15. *p*-Phenylphenol in Sodium *o*-Phenylphenate. Information would be requested from CEE on the necessity for such purity criteria.
16. Thiosulfate in Sodium Sulfites. The text would be prepared by Dr. EGAN for circulation.
17. Ascorbic Acid
18. Sodium and Calcium Ascorbates. The texts for methods 17 and 18 had been prepared by Prof. PELLERIN. The standards corresponded to a draft directive from CEE. This would be drawn to the attention of CEE.

In summary:

- (i) Methods 1, 3, 5, 7, 8, 10, 13, 14, 16, 17 and 18 would be circulated to Members of the Food Section and Commission on Analytical Reactions and Reagents.
- (ii) Method 6 would be circulated for further study in IUPAC.
- (iii) Method 4 would be held back by IUPAC.
- (iv) Methods for which information must be requested from CEE: 9, 11, 12 and 15. The attention of CEE would be drawn to the opportunity and necessity to do research on these methods. They would not be circulated in IUPAC until clarification had been received from CEE.
- (v) Methods 17 and 18 would be sent to CEE drawing their attention to the fact that these standards corresponded to a draft directive. The methods described and the standards retained were classical;

they appeared in the Codex Alimentarius or pharmacopoeas. Their inclusion was justified by the wish of CEE to finalize the antioxidants programme in 1973.

- (vi) The standards concerning butylhydroxyanisole (BHA) appeared in a CEE draft directive. Nevertheless, the study had not been undertaken. It appeared that the standards in this directive were not sufficient to ensure a satisfactory quality of BHA. IUPAC would draw the attention of CEE to this point.

Completion of 1973 Contract

The methods would be circulated as follows:—

- 1-20 April 1973: Despatch of methods by Dr. EGAN to Members of the Food Section and Commission on Analytical Reactions and Reagents.
- 15 June 1973: Last date for sending comments to Prof. PELLERIN.
- 1 July 1973: Collated report by Prof. PELLERIN to be sent to IUPAC Secretariat.
- 20 July 1973: Transmission of report by IUPAC Secretariat to all Members of the Food Section and Commission on Analytical Reactions and Reagents. Discussion of report at XXVII IUPAC Conference, Munich (August 1973).
- 1 October 1973: Final versions of methods ready for printing and transmission by Prof. TRUHAUT and Dr. EGAN to IUPAC Secretariat. Printed methods to be sent to CEE by 1 November 1973.

Any Other Business

Limit Test for Arsenic (25/72): The method would be revised by Mr. J. L. MONKMAN.

Further Studies

Chemical methods for traces of mercury, lead, and copper had been sent to CEE. It was envisaged that research on these trace metals would be by atomic absorption spectrophotometry. Dr. MARCUSE proposed to present research methods for these three elements by atomic absorption spectrophotometry. They would feature in the 1974 Contract. This study had been requested by CEE and its implementation was a function of the evolution of research.

Problems of Standardization

Dr. MARCUSE underlined the interest in standardization of international analytical methods for purity criteria of food additives; there was both national (notably Food Chemical Codex of USA) and international (FAO, IUPAC, Codex Alimentarius, *etc.*) interest. It was desirable to organize a roundtable conference allowing a wide exchange of views and which would lead to decisions for the coordination of standardization efforts. This meeting could be organized in Hamburg on 30 August 1973 during the IUPAC-IUFoST Symposium.

Prof. TRUHAUT would try to obtain the agreement of CEE to the organization of a roundtable meeting and if the response was positive, send an official invitation to that organization to be represented. Meanwhile, Dr. MARCUSE would make contact with other international organizations thought to be interested.

R. TRUHAUT

REPORTS OF IUPAC-SPONSORED SYMPOSIA

INTERNATIONAL SYMPOSIUM ON SELECTIVE ION-SENSITIVE ELECTRODES

Cardiff, 9-12 April 1973

This Symposium, held in the Chemistry Department of University of Wales Institute of Science and Technology (UWIST) and attended by about 200 delegates, had an international flavour with participants from Belgium, Czechoslovakia, Denmark, France, Germany, Hungary, Israel, Italy, Japan, Poland, Portugal, Romania, South Africa, Sweden, Switzerland, UK, USA.

All the most relevant aspects of selective ion-sensitive electrodes were covered in five plenary lectures (to be published in the official IUPAC journal, *Pure and Applied Chemistry*) and sixty papers. A special bound copy of the abstracts is available from the Short Course Organizer at UWIST.

The wide variety of materials which had been utilized in precipitate-based selective ion-sensitive electrodes was summarized by Prof. E. PUNGOR (Hungary) in the opening plenary lecture. The functional parameters and uses of some silicone rubber electrodes by the Pungor school were described in six short papers.

The current state of thinking on the mechanistic aspects of selective ion-sensitive electrodes was succinctly presented in the second plenary lecture by Prof. G. A. RECHNITZ (USA), who emphasized the urgent need for a considerable research effort in this area. Papers on recent mechanistic studies were introduced by Prof. O. KEDEM (Israel); Prof. P. R. DANESI (Italy); Prof. R. P. BUCK (USA); Dr. K. GARBETT (UK); Dr. J. A. W. DALZIEL (UK); and Dr. B. KARLBERG (Sweden).

The next plenary lecture by Prof. W. SIMON (Switzerland) surveyed the important research of the Zürich group on selective ion-sensitive electrodes, embracing crown compounds, valinomycin and other antibiotics in polyvinyl chloride matrices. A new electrode for calcium proved superior to any commercial model particularly regarding operational lifetime. Dr. J. PETRÁNEK (Czechoslovakia) discussed the interference of sodium for potassium electrodes based on eleven different crown compounds immobilized in polyvinyl chloride sensor matrices.

Selective ion-sensitive electrodes measured the activities *not* concentrations of ions. Prof. R. G. BATES (USA) elaborated on the most recent concepts of ion activity scales which were of such fundamental thermodynamic significance. This excellent plenary lecture was backed up in the subsequent papers by Dr. R. A. DURST (USA); Dr. J. PADOVA (Israel); Dr. J. JANATA (UK); Dr. T. H. LILLEY (UK); Dr. A. TATEVOSSIAN (UK); Dr. M. WHITFIELD (UK); Prof. G. MILAZZO (Italy); and Dr. C. FUCHS (Germany).

The final plenary lecture, delivered in two parts by Dr. J. W. ROSS (USA) and Dr. R. H. RISEMAN (USA), dealt with the theoretical and practical aspects of sensor electrodes developed for several common gases. Two other papers by Dr. D. MIDGLEY (UK) and Dr. J. MERTENS (Belgium), respectively, detailed their application for continuously monitoring carbon dioxide and ammonia in boiler-feed waters.

A wide choice of the applications of selective ion-sensitive electrodes was offered on the following topics: the solubility products of lanthanide fluorides (Dr. J. J. R. FRAÚSTO DA SILVA, Portugal); the stability constants of metal-

ligand systems (Dr. E. HANSEN, Denmark; Prof. K. L. CHENG, USA; and Dr. J. J. R. FRAÚSTO DA SILVA, Portugal); fluoride assays (Dr. A. HENRION-BOECKSTIJNS, Belgium; Dr. A. TATEVOSSIAN, UK; and Dr. B. SCHREIBER, Switzerland); halide assays (Dr. G. J. KAKABADSE, UK; and Dr. E. J. DUFF, UK); the level of cyanide and metal ions in plating baths, (Dr. L. ŠUCHA, Czechoslovakia); continuous online analysis (Dr. B. FLEET, UK; and Dr. J. N. ANGEL, UK); enzyme assay (Prof. M. MASCINI, Italy); medical problems (Dr. D. A. STANLEY, UK; Dr. J. LADENSON, USA; and Prof. C. E. SACHS, France); free energy measurements, (Dr. A. K. COVINGTON, UK) and fused salt baths (Dr. J. MESPLEDE, France; Dr. R. COMBES, France; and Dr. W. J. DE WET, South Africa).

The construction and evaluation of miscellaneous electrodes were described for PVC- or filter paper-liquid ion exchanger membranes by Dr. G. J. MOODY (UK); Dr. M. LESKO (Poland); and Dr. A. HULANICKI (Poland); graphite-Selectrodes by Dr. J. RŮŽIČKA (Denmark); and Dr. J. R. ENTWISTLE (UK); organic radical ions by Dr. M. SHARP (Sweden); and ion association systems for maleate and phthalate ions by Dr. N. ISHIBASHI (Japan).

The design and performance of micro electrodes employing the liquid ion-exchanger in drawn glass capillaries or in PVC coated wires were discussed by Dr. J. L. WALKER (USA); Dr. J. R. COCKRELL (USA); Dr. J. HAVAS (Hungary); and Dr. G. J. MOODY (UK).

Some important aspects of the calibration format essential to the performance of electrodes were treated by Dr. R. J. SIMPSON (UK). The thermal properties of several electrodes were discussed by Dr. T. S. LIGHT (USA) and by Dr. F. O. OEHRME (Switzerland).

Dr. D. JAGNER (Sweden) reviewed the precision and accuracy associated with Grans plots for known addition and subtraction techniques.

G. J. MOODY

IV INTERNATIONAL CONFERENCE ON SOLID COMPOUNDS OF TRANSITION ELEMENTS

Geneva, 9-13 April 1973

The I International Conference on Solid Compounds of Transition Elements was held in Paris-Orsay in 1965. Since then it has become an established tradition to hold a Conference in the series every 2 or 4 years. The II Conference was held at the Technical University of Twente in Enschede in 1967 and the III Conference took place at the University of Oslo in June 1969. These Conferences are a supplement to the more general ones on crystallography, magnetism, semiconductors, *etc.* Like the preceding ones, the Geneva Conference was concerned with the physical and chemical properties of solid compounds of transition elements, especially those containing sulfur, selenium, tellurium, nitrogen, phosphorus, arsenic, antimony, and bismuth. The aim of the Conference was to bring together chemists and physicists who are actively contributing to our knowledge and understanding of the structural, electrical, magnetic, thermodynamic, and other relevant physicochemical properties of these compounds.

The IV Conference was held at the School of Physics of the University of Geneva under the sponsorship of IUPAC, IUPAP, European Physical Society, Société Suisse de Physique, Société Suisse de Chimie, and Société Suisse de Cristallographie. The Conference was organized by Prof. E.

PARTHÉ and the members of the Laboratoire Interdisciplinaire de Cristallographie aux Rayons X of the University of Geneva. Direct or indirect financial support had been offered by IUPAP, the City and Canton of Geneva, the Science Faculty of the University of Geneva, Battelle Geneva Research Centre, and N.V. Philips Gloeilampenfabrieken in Eindhoven and Zürich.

About 200 participants from 17 different countries, one third of them from France, were attracted to the meeting. Seventy papers were submitted for presentation. The extended abstracts of these papers were bound and given to each participant at the beginning of the Conference. Five speakers were especially invited to this Conference: Prof. A. NECKEL (Technical University in Vienna) spoke on the electronic structure of transition metal carbides and nitrides. Dr. M. H. LEWIS (University of Warwick in Coventry) opened a session with his talk on ordered vacancy arrangements in transition metal carbides and nitrides. Following the invited lecture given by Dr. R. FRUCHART (CNRS Laboratory in Vitry/Seine) on the structural evolution of the phosphides and arsenides M_2X , were scheduled 6 papers on magnetic, Mössbauer, and structural studies on Fe_2P or Fe_2As . Laboratories in France, Sweden, and Belgium had investigated the same properties independently and obtained different results. It appears now that minute changes in the chemical composition can have drastic effects on the physical properties of these compounds. Dr. E. BUCHER (Bell Laboratories in Murray Hill), with his contribution on magnetism and related electronic properties of Pm and Tm binary chalcogenides, started off the two-day session on the physical properties of the chalcogenides. The fifth invited speaker, Dr. A. JAYARAMAN (also from the Bell Laboratories), opened the session on rare earth compounds with his talk on pressure-induced semiconductor-metal transitions in bivalent rare earth monochalcogenides.

One morning was reserved for a visit to CERN, the European Centre for Nuclear Research. A reception for the Conference participants was offered by the City and Canton of Geneva in the foyer of the Grand Théâtre of Geneva. A second reception was given by the Battelle Geneva Research Centre. The social highlight of the conference was the closing banquet, a candlelight dinner in the Salle de Justice of the medieval Château de Chillon near Montreux on the lake of Geneva.

E. PARTHÉ

INTERNATIONAL CONFERENCE ON EDUCATION OF TEACHERS FOR INTEGRATED SCIENCE

University of Maryland, USA: 3-13 April 1973

The Conference—with the theme 'Teaching Science for Today's Society'—was organized by the ICSU Committee on Teaching of Science in collaboration with UNESCO, the US National Commission for UNESCO, and the University of Maryland.

The programme was concerned with the interdisciplinary approach to science education at primary and secondary level, and followed up the work of the Varna Conference in 1968 where the central question was 'Why integrate the teaching of science?' The major aspect of this Conference was the education of teachers—both initial and in-service—to teach science in both integrated and coordinated ways.

The Conference stimulated a remarkable interest. More than 200 participants from 63 countries from all parts of the world attended. The Conference was commended by several distinguished scientists, including Nobel Laureates, who in their letters of support, expressed very great sympathy for the ideas discussed.

The participants were welcomed by Prof. F. STAFLEU, Secretary General of ICSU, and other distinguished scientists representing the highest scientific authorities in USA presented short papers. These included Dr. W. ELKINS, President of the University of Maryland, and Dr. L. REISER, President of the American Association for Advancement of Science. A reception for participants was given by the US State Department and the US National Commission for UNESCO.

The structure of the Conference consisted of plenary sessions where invited papers were read followed by some discussion, and eight working groups where selected topics were discussed in greater depth. In this way all participants were actively involved in the Conference. The conclusions of the working groups were summarized in a final report which, together with summaries of the plenary session papers, constitute the Conference Report. The Proceedings of the Conference, comprising fuller versions of the main papers and extended reports of the working groups, will be published in the Spring of 1974 by UNESCO in the *New Trends* series (these volumes may be ordered through booksellers or from UNESCO). The Conference Report may be obtained from the Secretary, ICSU Committee on Science Teaching [CEDO, Tavistock House South, Tavistock Square, London WC1H 9LL, UK, at the price of \$1.25 (50p), including postage (payable in advance: cheques, etc., made out to ICSU Committee on Science Teaching)].

The principal subjects under discussion included: Integrated Science and Teacher Education; Desirable Characteristics and Competencies of Teachers of Integrated Science; New Approaches to Preparation and In-Service Teaching of Teachers—New Materials for Education of Science Teachers and Role of Laboratory Experience; Contributions of Courses other than those in Science; Open University Courses in Science and Technology Applicable to Education of Teachers of Integrated Science; Evaluation of Programmes for Education of Teachers of Integrated Science; Social Responsibility of Scientists and Reciprocal Responsibility of Society; Social Significance of Teaching of Science and Mathematics; Reorientation of

Specialists for a Role in Teaching of Integrated Science; Role of Science Teaching Centres in Preparation of Teachers of Integrated Science.

The Conference was followed by a two-day meeting (13-15 April 1973) at which representatives of Science Teachers' Associations prepared the way for the formation of an International Council of Associations for Science Education. Such an organization will aim at extending and improving education in science for all children and young people throughout the world and would be particularly concerned to provide means of communication among member Associations.

Initially, some nineteen Science Teachers' Associations from seventeen countries will be members of the International Council. The first task of the elected Executive Committee is to invite further Science Teachers' Associations or members of science education sections of national scientific bodies to take part in the activities of the International Council. Dr. J. D. LOCKARD (University of Maryland) was elected as President in his capacity as the representative of the National Association for Research in Science Teaching. The Executive Secretary is Mr. D. G. CHISMAN, Secretary of the ICSU Committee on Science Teaching.

D. G. CHISMAN

Official Representative of IUPAC to
ICSU Committee on Teaching of Science

FORTHCOMING IUPAC PUBLICATION FROM BUTTERWORTHS

STANDARD METHODS FOR ANALYSIS OF OILS, FATS, AND SOAPS

The following methods have recently been adopted and edited for publication by the Section on Oils and Fats:

- II.C.6 Determination of the Phosphoric Acid Test (PAT) Value of Raw Linseed Oil
- II.C.7 Determination of Mono-, Di-, and Triglycerides by Column Chromatography
- III.A.3 Determination of Water in Glycerol (Karl Fischer Method)
- III.A.4 Determination of Ash in Crude Glycerol
- III.A.5 Determination of Alkalinity or Acidity of Crude Glycerol
- III.A.6 Calculation of MONG in Crude Glycerol

These methods are additional to those included in the 5th Edition (1964) and its two Supplements (1966, 1973).

Available early in 1974.

FORTHCOMING IUPAC-SPONSORED SYMPOSIA

II IUPAC CONFERENCE ON PHYSICAL ORGANIC CHEMISTRY

Noordwijkerhout, 29 April-2 May 1974

At the XXIV IUPAC Conference in Cortina d'Ampezzo (1969), the Organic Chemistry Division proposed to start a regular series of meetings on physical organic chemistry in alternate years. The first Conference was held in 1972 at Crans sur Sierre in Switzerland. The second Conference, sponsored by IUPAC and the Royal Netherlands Chemical Society, will be held in 'De Leeuwenhorst' at Noordwijkerhout. The Leeuwenhorst is situated close to the North Sea coast amidst the bulb fields, near Leiden (10 km), Amsterdam (35 km), and Schiphol international airport (25 km).

Scientific Programme

The programme of this Conference will emphasize important developments in the study of reaction mechanisms and related areas. The Conference language will be English.

Plenary Lecturers

Plenary lectures will be given by:

R. BRESLOW
O. L. CHAPMAN
M. JULIA
G. G. HAMMES

E. HEILBRONNER
R. SUSTMAN
S. TRIPPETT

and they will eventually be published in *Pure and Applied Chemistry*, the official journal of IUPAC.

Contributed Papers

The programme will allow for the presentation of a limited number of contributed papers on topics directly related to that of the Conference. Participants who wish to present such a paper, are invited to indicate this as soon as possible. The abstract should reach the Organizers not later than 30 November, 1973. Abstracts should be typewritten according to the rules of *Tetrahedron Letters* concerning size, title, names of authors and institutes, etc.

Correspondence

All correspondence concerning the Conference should be addressed to:

Prof. TH. J. DE BOER
Laboratorium voor Organische Scheikunde
Universiteit van Amsterdam
Nieuwe Achtergracht 129
Amsterdam, Netherlands

The number of active participants will be restricted to about 250. In the case of more applications, the Organizing Committee is entitled to make a selection of participants.

IX INTERNATIONAL SYMPOSIUM ON CHEMISTRY OF NATURAL PRODUCTS

Ottawa, 24-28 June 1974

The Symposium will be held at Carleton University, Ottawa. Accommodation will be available in the University residences and local hotels. Many government research laboratories are located in the city. In addition, Ottawa, Canada's capital, offers many attractions for the visitor.

Invited Lectures

There will be a number of invited lectures by distinguished scientists. The main lectures delivered at the Symposium will be published in *Pure and Applied Chemistry*, the official journal of IUPAC, and also made available as a specially bound reprint.

Contributed Papers

The Programme Committee will consider papers of special interest and novelty in natural products chemistry within the following areas:

- (a) Total synthesis of natural products
- (b) Transformations of natural products
- (c) Structures and properties of natural products
- (d) Natural products of medicinal interest
- (e) Bioorganic chemistry
- (f) Marine and insect chemistry

Symposium Language

The official languages of the Symposium will be English and French. Contributed papers may be presented in any language but the organizers suggest that speakers should, as far as possible, use English or French. No arrangements will be made for simultaneous translation. Symposium literature will be published in English and French.

Ladies Programme, Social Events, Technical Tours

Various functions will be arranged for those accompanying registered participants as well as for those attending the Symposium.

Pre- and/or Post-Symposia

Preliminary plans have been made to arrange two pre- and/or post-symposia of restricted scope, with a limited number of participants.

Secretariat

Please address communications to:

M. K. WARD, Executive Secretary
IX International Symposium on
Chemistry of Natural Products
c/o National Research Council of Canada
Ottawa, K1A 0R6, Canada

III INTERNATIONAL CONGRESS OF PESTICIDE CHEMISTRY

Helsinki, 3-9 July 1974

The Congress will be held at Finlandia Hall, Helsinki's new congress and music centre. The Hall is situated near the Parliament House in the centre of the city.

Scientific Programme

In the scientific programme of the Congress, insecticides, fungicides, herbicides, other pesticides, and related substances will be discussed under ten main topics which are divided into a number of subtopics. The titles of the subtopics are tentative and subject to changes in the final programme according to the nature of the papers submitted.

1. *Pesticide residue analysis*
 - (a) Sampling, sample processing, and extraction procedures for residue analysis
 - (b) Automation of analysis (a symposium in preparation)
 - (c) Methodology of analysis (multiresidue and specific)
 - (d) Interfering substances in analysis (PCBs, etc.)
 - (e) Instrumental and bioassay techniques for analysis of herbicide residues (a symposium in preparation)
2. *Pesticide residues in food and feed commodities and total diets*
 - (a) Chemical nature of terminal pesticide residues
 - (b) Pesticide residues in food and feed commodities moving in commerce
 - (c) Fate of pesticide residues in processing and storing of food and feed
 - (d) Pesticide residues in total diets
 - (e) Effects of pesticide residues on chemical composition of plant products
3. *Impact of environmental factors on chemical behaviour of pesticides in plants, soils, and waters*
 - (a) Effect on physicochemical behaviour of pesticides
 - (b) Effect on metabolism of pesticides
 - (c) Effect on disappearance rate of pesticide residues
4. *Relationship of chemical structure to biological activity of pesticides*
 - (a) Systemic action
 - (b) Mode of action, synergism, and antagonism
 - (c) Selectivity
 - (d) Adaptation chemistry of organisms to pesticides (a symposium in preparation)
5. *Pesticides in cell metabolism*
 - (a) Membrane permeability
 - (b) Mechanisms of biotransformation of pesticides
 - (c) Implications in metabolism
6. *Pesticide toxicology and pharmacology*
 - (a) Biochemical and metabolic behaviour of pesticides in man and animals
 - (b) Measurement and toxicological evaluation of pesticide loads in man and animals.
 - (c) Toxicological effects of accidental and occupational exposure of man to pesticides

- (d) Recommendations for acceptable levels of daily exposure of man to pesticides (tolerances, etc.; a symposium in preparation)
- 7. *Chemistry and activity of naturally occurring pestidical compounds and related substances*
 - (a) Pesticides of plant origin (a symposium in preparation)
 - (b) Pesticides of microbiological origin
 - (c) Viruses
 - (d) Insect pheromones and hormones
 - (e) Insect chemosterilants
 - (f) Insect repellents
- 8. *Industrial aspects of pesticide chemistry*
 - (a) New pesticides (chemistry, properties, and activity)
 - (b) Formulation chemistry
 - (c) Industrial technology
 - (d) Waste problems
- 9. *Pesticide legislation in various countries*
- 10. *National, regional, and global statistics on use of pesticides*

Special Symposium

In connection with the Congress a special IUPAC Symposium on *Dispersion Dynamics of Pollutants in the Environment with Special Reference to Pesticides* will be held on 5-6 July.

The Symposium is being organized jointly by the Institute of Occupational Health, Helsinki, Finland, and the Institute of Ecological Chemistry, Schloss Birlinghoven, German Federal Republic. The following main topics will be discussed:

- 1. *Transport mechanisms of pesticides in air, water, soil, and biosphere*
- 2. *Monitoring for environmental pesticide pollutants*
- 3. *Case studies of dispersion of pesticide pollutants in various geographical areas (e.g., Baltic Sea)*
- 4. *Transference of environmental pesticide pollutants into microbes, wild-life, and man.*

Features of Technical Programme

The technical programme of the Congress will consist of plenary sessions, symposia, and general sessions on papers submitted.

Plenary Sessions

In the plenary sessions of the Congress seven 45-minute lectures will be given. The speakers and their subjects (tentative or final) are as follows:

Prof. R. D. O'BRIEN (USA)	The Forces which Bind Insecticides to their Targets (tentative)
Dr. H. FREHSE (German Federal Republic)	Problems and Aspects of Present-day Residue Analysis
Dr. C. A. EDWARDS (UK)	Factors that Influence Persistence of Pesticides in Plants and Soils
Dr. H. HURTIG (Canada)	Transformation and Fate of Pesticide Residues in Food Storage and Processing (tentative)
Prof. K. MUNAKATA (Japan)	Insect Antifeeding Substances in Plant Leaves

Dr. E. KNÜSLI
(Switzerland)

One lecture from USSR (open)

The Future of the Development of Pesticides
by Industry

Symposia

A number of symposia will be organized on subjects of special interest which relate to the main topics of the Congress. Some symposia are in preparation and some will be arranged on the basis of proposals herewith requested and made in due time to the Scientific Programme Committee.

A symposium is preferably half a day long (3 hours) and only exceptionally a full day (6 hours). The lectures are given by invited speakers. The duration of one lecture is not more than 20 minutes. In order to give time for open discussions, five lectures can regularly be scheduled for one 3-hour symposium.

Some time is reserved in symposia for short communications submitted to the Congress and related to the subject of a symposium. The short communications are read by the authors or summarized by the chairman.

General Sessions on Papers Submitted

Any participant may offer a short communication not previously published for the programme of the Congress and the Special Symposium. These communications are given either in symposia (see above) or in general sessions of papers submitted. The general sessions are organized according to the topics on the programme and the nature of papers submitted. A total of 15 minutes including discussions is allotted for the presentation of a paper in a general session.

The short communications are placed on the programme of the Congress and the Special Symposium on the basis of abstracts submitted in due time to the Scientific Programme Committee.

In order to avoid excessive expansion of the programme it may become unavoidable to limit the number of papers scheduled on the programme. Preference in acceptance will be given to papers which are closely related to the topics of the Congress and the Special IUPAC Symposium and which emphasize new chemical achievements in pesticide science. The authors of the abstracts of the short communications will be notified about the acceptance and placement of their papers on the programme.

Special IUPAC Symposium

The technical programme of the Special IUPAC Symposium will consist of about fifteen 40-minute lectures given by invited speakers, of short communications, and of open discussions.

Short communications submitted to the Symposium and accepted by the Organizing Committee will be given either in full by the authors in the general sessions or summarized by the chairman at the relevant sessions (see General Sessions on Papers Submitted).

The following invited speakers have confirmed their intention to appear on the programme of the Symposium:

Prof. H. FLOHN (German Federal Republic)	Natural Longterm Changes of Global Environment
Prof. CHR. JUNG (German Federal Republic)	Transport Mechanism in Air
Prof. A. M. AITSAM (USSR)	Transport Mechanism in Water
Prof. E. P. LICHTENSTEIN (USA)	Transport Mechanism in Soil

Prof. L. J. MEDVED (USSR)	Transport Mechanism in Biosphere
Dr. P. BAGGE (Finland)	Case Presentation: The Baltic Sea
Dr. A. LAAMANEN (Finland)	Optimization Procedures for Environmental Sampling in Space and Time
Dr. J. ROBINSON (UK)	Mathematical Models
Dr. A. R. BARRINGER (Canada)	Remote Sensing Techniques
Prof. F. COULSTON (USA)	Mutagenic Carcinogenic, and Teratogenic Effects of Pollutants with Respect to Man

Publication of Papers

Abstracts of plenary lectures, symposium lectures, and short communications will be made available to the registered participants before the Congress.

Publication rights are retained on all papers given at the Congress and the Special IUPAC Symposium. The plenary lectures, symposia lectures, and short communications will be published in full after the Congress. The deadline for submitting the full manuscripts of the papers to be given at the Congress is 15 May 1974. Detailed instructions will be given later.

Congress Language

The official language of the Congress is English. No simultaneous translation will be provided in the sessions. Abstracts and manuscripts must be written in English.

General Information

Travel

It is easy to reach Helsinki. There are frequent direct flights from many European cities and USA, luxurious car ferries from Sweden, Denmark, German Federal Republic, and Poland, and trains from USSR. The roads are good for travelling by car.

Charter and group flights from various countries are under consideration. Further information will be provided on request by the secretariat of the Congress.

Finnair, as the official carrier of the Congress, is prepared to offer the best possible cooperation through its local agencies.

Accommodation

The hotels are at walking distance from Finlandia Hall. Arrangements are also being made for accommodation in inexpensive, but very acceptable, summer hotels, which can be reached by bus.

Touring and vacationing

Sightseeing and post-congress tours to different parts of Finland will be organized. There are good connections with the other Nordic countries and USSR for more extended tours. July is an ideal month for vacationing in Finland. Many guests may be interested in spending some time in holiday resorts.

Correspondence

All correspondence should be addressed to the Secretary General:

Dr. J. LARINKARI
Federation of Finnish Chemical Industry
POB 28
SF-00131 Helsinki 13
Finland
Telephone: Finland 90-10 300
Cable: Chemcongress, Helsinki

INTERNATIONAL SYMPOSIUM ON MACROMOLECULES

Rio de Janeiro, 26-31 July 1974

The Brazilian Academy of Sciences, the National Research Council of Brazil and the Science and Technology Secretariat of Guanabara State are pleased to invite participation in the International Symposium on Macromolecules—SIM—to be held in Rio de Janeiro, Guanabara, under the sponsorship of IUPAC. The Symposium will take place in the Hotel Nacional-Rio.

Topics

Symposia will be held on topics to be selected from such important areas in science and technology as the following:

- 1—Solution and bulk properties of polymers
- 2—Polymer characterization methods
- 3—Homo- and copolymerization reactions
- 4—Photopolymerization
- 5—Chemical reactions on macromolecules
- 6—Evaluation of polymer properties
- 7—Advances in polymer technology
- 8—Natural polymers—reactions and technology
- 9—Advances in biopolymers and their synthetic models

Contributed Papers

Contributed papers in the general fields covered by the mentioned symposium topics will be accepted. Contributors should indicate in their application to which symposium field the paper is most closely related. The Programme Committee may accept contributed papers of exceptional interest on subjects other than those listed. The abstracts are requested to be in English and of no more than 250 words. At the opening of SIM a volume containing the abstracts of the accepted papers will be distributed to all participants.

Symposium Languages

The official language of SIM will be English, though papers may be presented either in English or in any of the following languages, for which there will be simultaneous translation into English: Portuguese, Spanish, Italian, French, and German.

Correspondence

Enquiries and other correspondence concerning the Symposium should be addressed to:

Prof. ELOISA BIASOTTO MANO
Simpósio Internacional de Macromoléculas
Academia Brasileira de Ciências
Caixa Postal 229
20.000 Rio de Janeiro, GB
Brazil

IV INTERNATIONAL SYMPOSIUM ON MEDICINAL CHEMISTRY

Noordwijkerhout, 9-13 September 1974

At the meeting in Milan in 1972 of the European Federation of Medicinal Chemistry, it was decided, in agreement with the IUPAC Section on Medicinal Chemistry, to start a regular series of International Medicinal Chemistry Symposia in alternate years. Preceding symposia were held in Florence (1962), Münster (1968), and Milan (1972).

The fourth International Symposium on Medicinal Chemistry will be held in the 'Congress Centre Leeuwenhorst' at Noordwijkerhout. The Leeuwenhorst is situated close to the North Sea coast near Leiden (10 km), Amsterdam (35 km), and Schiphol international airport (25 km). It offers its guests a pleasant stay in a well-run establishment, still retaining an atmosphere of rural peace and quietness.

The meeting is being organized by the Medicinal Chemistry Division of the Royal Netherlands Chemical Society in cooperation with the Medicinal Chemistry Division of the Flemish Chemical Society, under the sponsorship of IUPAC (Section on Medicinal Chemistry), Fédération Internationale Pharmaceutique, Royal Netherlands Chemical Society, and Royal Netherlands Association for the Advancement of Pharmacy.

Scientific Programme

The topics selected so far for the scientific programme are:

1. Medicinal Chemistry of Thrombolytic and Antithrombotic Agents
2. Medicinal Chemistry related to Central Transmitters
3. Chemical Structure and Pharmacokinetics

A basis for the modulation of therapeutic and toxic action

4. Chemotherapy of Parasitic Infections
Antiprotozoal agents and anthelmintics

The symposium language will be English.

Plenary Lectures

About fifteen lecturers will be invited (speaking-time 45 minutes). To date the following speakers have accepted:

Topic 1: Dr. P. BRAKMAN (Netherlands), Dr. J. A. DURDEN, Jr. (USA), Dr. D. MILLS (USA), Prof. D. P. THOMAS (UK).

Topic 2: Prof. H. CORRODI (Sweden), Prof. Dr. D. G. GRAHAME-SMITH (UK), Dr. M. SANDLER (UK), Dr. H. STÄHLE (GFR)

Topic 3: Prof. E. J. ARIËNS (Netherlands), Prof. E. J. LIEN (USA), Prof. A. H. BECKETT (UK)

Topic 4: Dr. E. F. ELSLAGER (USA), Dr. H. LOEWE (GFR)

Communications

The programme will allow for the presentation of short communications (15 minutes, discussion included) and a small number of 30-minute lectures for which the Organizing Committee can extend an invitation. The communications, which will be subjected to a selection procedure, should be related directly to the symposium topics.

Publication of Symposium Papers

The full text of invited lectures will eventually be published in a volume of symposium proceedings.

Application for Participation

The number of active participants is restricted to about 450. Participants will be accommodated in 'Leeuwenhorst'.

Correspondence

Enquiries and other correspondence should be addressed to the Symposium Secretariat:

MERCK SHARP & DOHME BV
Professional and Government Liaison
Waarderweg 39
POB 581
Haarlem, Netherlands

II SYMPOSIUM ON INORGANIC PHOSPHORUS COMPOUNDS

Prague, 10-14 September 1974

The Symposium will be held at the Institute of Chemical Technology, Prague-Dejvice. It is being organized, under the sponsorship of IUPAC, by the Czechoslovak National Committee for Chemistry, Czechoslovak Chemical Society, and Prague Institute of Chemical Technology, in collaboration with the Department of Chemistry of the Pedagogical University in Ústí nad Labem, Department of Inorganic Chemistry of Charles University in Prague, Department of Inorganic Chemistry of J. E. Purkyně University in Brno, and Department of Inorganic Technology of Slovak Technical University in Bratislava.

Scientific Programme

The scientific programme will consist of an invited lecture on each of the topics in the following subject groups, and contributed papers:

1. Elementary Phosphorus and Lower Valency Compounds of Phosphorus
2. Monomeric and Polymeric Phosphates and their Derivatives
3. Phosphorus-Nitrogen Compounds
4. Phosphorus in Ligands of Coordination Compounds
5. Organoderivatives of Inorganic Phosphorus Compounds
6. Halides and Chalkogenides of Phosphorus
7. Chemical Bond and Molecular Structure of Inorganic Phosphorus Compounds

8. Spectroscopic Methods in Phosphorus Chemistry
9. Chromatography of Phosphorus Compounds
10. Physicochemical and Analytical Methods in Chemistry of Phosphorus Compounds
11. New Applications of Inorganic Phosphorus Compounds

A limited number of contributed papers, not exceeding 15 minutes reading time, will be registered.

The main lectures delivered at the Symposium will be published in *Pure and Applied Chemistry*, the official journal of IUPAC, and also made available as a specially bound reprint.

The official languages of the Symposium are English, Russian, German, and French.

Other Information

A programme of social events and an exhibition of chemicals, laboratory instrumentation, technological equipment, and literature is being planned.

From 17 to 21 September 1974 an International Symposium on Organophosphorus Compounds will be held in Torun (Poland). This meeting will immediately follow the Symposium in Prague and will be organized in collaboration with it.

Correspondence

The address of the Symposium Secretariat is:

Department of Inorganic Chemistry
Prague Institute of Chemical Technology
Suchbátarova 5
CS-166 28 Praha-Dejvice
Czechoslovakia
Telephone: 320 249

II INTERNATIONAL SYMPOSIUM ON CHEMISTRY OF NONBENZENOID AROMATIC COMPOUNDS

Lindau/Bodensee, 23-27 September 1974

The Symposium is being organized by Gesellschaft Deutscher Chemiker under the sponsorship of IUPAC.

Scientific Programme

The Organizing Committee wishes to present a programme consisting of novel and important developments in the chemistry of nonbenzenoid aromatic compounds excluding common heteroaromatics. Submitted papers should deal with the chemistry, properties, and structure, as well as theoretical studies of nonbenzenoid aromatic compounds.

There will be twelve invited plenary lectures. The following chemists have accepted invitations to give these lectures:

- | | |
|----------------------------|--|
| Prof. A. G. ANASTASSIOU | Synthesis and Study of Select Heterocycles |
| (USA) | |
| Prof. V. BOEKELHEIDE (USA) | Intrusion of Substituents into the Cavity of Aromatic π -Electron Clouds |

Prof. M. J. S. DEWAR (USA)	MO Studies of Some Nonbenzenoid Aromatic Systems
Dr. P. GARRATT (UK)	Polycyclic Systems containing Small Membered Rings
Prof. H. GÜNTHER (Federal Republic of Germany)	Results of ^{13}C -NMR Spectroscopy in the Field of Cyclic Conjugated π -Electron Systems
Prof. E. HEILBRONNER (Switzerland)	Photoelectron-spectra of Nonbenzenoid Cyclic Conjugated π -Electron Systems
Prof. Y. KITAHARA (Japan)	Oxoheptafulvene
Prof. S. MASAMUNE (Canada)	Degree of Electron Delocalization in Some Small-ring Systems
Prof. M. NAKAGAWA (Japan)	Acetylene-Cumulene-Dehydroannulenes
Prof. J. F. M. OTH (Switzerland)	π -Bond Situation (Delocalization or Localization) in Annulenes and their Ions
Prof. G. SCHRÖDER (Federal Republic of Germany)	Higher-membered Annulenyl Ions
Prof. R. ZAHRADNIK (CSSR)	Electronic Structure of Radical Ions and Diions Derived from Nonalternant Systems

The invited plenary lectures will be published in *Pure and Applied Chemistry*, the official journal of IUPAC.

Symposium Language

The invited plenary lectures will be given in English. Other contributed papers may be presented in any IUPAC language, but the organizers hope that the speakers will use English. No arrangements will be made for translation.

Contributed Papers

Participants who wish to present a paper at the symposium are invited to indicate this not later than 31 December 1973. Only a limited number of short papers (15 minutes) can be presented during the Symposium. Therefore, it may become necessary to make selections. The Organizing Committee will have the final responsibility for acceptance of the papers. Authors will be informed before the end of April 1974 whether their papers have been accepted. Abstracts of papers to be presented will be distributed to participants on registration.

Correspondence

All correspondence concerning the symposium should be addressed to:

Dr. W. FRITSCHÉ, General Secretary
Gesellschaft Deutscher Chemiker
D-6000 Frankfurt (M) 8
Postfach 119075
Federal Republic of Germany

SPONSORSHIP OF SYMPOSIA BY IUPAC

Advance Information

IUPAC reserves the right to publish in its official journal, *Pure and Applied Chemistry* (or in book form), the whole or part of the proceedings of any symposium or congress which it sponsors. The publication of proceedings of a meeting cosponsored with another organization shall be the subject of special arrangements. Because a decision on sponsorship is taken only after the question of publication has been carefully considered, the Bureau requires advance information about symposia. Organizers of meetings who are considering making an application for sponsorship should supply the necessary information for consideration by IUPAC preferably two years before the actual meeting.

This information is most conveniently supplied in the form of answers to an Advance Information Questionnaire, copies of which can be obtained from the Executive Secretary (IUPAC Secretariat, Bank Court Chambers, 2-3 Pound Way, Cowley Centre, Oxford OX4 3YF, UK).

Scope of Publication

Organizers should plan to make available to IUPAC 6-12 main (plenary or sessional) lectures, some of which should survey critically the state of the particular field of research, giving pointers to future work: summaries or reports of discussions are not normally published. The Bureau will, however, consider carefully any requests for departures from this general policy. Organizers of sponsored meetings are free to make their own arrangements for the publication of any part of the proceedings which IUPAC decides not to publish.

Preparation and Collection of Manuscripts

It is a condition of granting sponsorship to a symposium, the proceedings or part of which will be published by IUPAC, that the Organizers shall appoint a senior person as Symposium Editor well in advance of the symposium. Manuscripts for publication will be collected by the Symposium Editor, preferably no later than at the actual meeting. After completing his other responsibilities (detailed in 'Notes for IUPAC Officers and Organizers of Meetings'*) the manuscripts should be sent immediately to the Union's Scientific Editor. As far as possible, papers should conform to the general style set out in 'Notes to Contributors'.*

Freedom of Participation

Organizers of meetings to be under the auspices of IUPAC, in considering the location of such meetings, should take all possible steps to ensure the freedom of all *bona fide* chemists to attend. Unless such provision is made, IUPAC may find it impossible to grant sponsorship.

*Available from IUPAC Secretariat.

Subvention

Requests for subvention to meetings granted sponsorship by IUPAC should be made to the IUPAC Secretariat. Save in special circumstances, the granting of subvention will be limited to symposia which are to be held in non-IUPAC conference years.

Organizers requesting subvention will be asked to supply a draft realistic budget. As a general principle, IUPAC regards elaborate and expensive social events at symposia as undesirable. The cost of such events should not be included in the registration fee, which might hinder the attendance of young chemists. Social events should be self-supporting and not require financial help from IUPAC. Also, subvention from the union should not be used for the hiring of meeting rooms.

FINAL REPORTS FROM IUPAC

The following Final (Definitive) Reports have recently been published in *Pure and Applied Chemistry*:—

1. A Collaborative Study of Dynamic, Mechanical and Impact Properties of PVC-II (Macromolecular Division): **35** (3), 315.
2. Definitive Recommendations for Presentation of Raman Spectra for Cataloging and Documentation in Permanent Data Collections (Commission on Molecular Structure and Spectroscopy): **36** (1-2), 277.

Subject to the prior agreement of IUPAC, the definitive recommendations in Report 2 may be:

- (a) Republished in the journals of National Adhering Organizations and National Societies (but not of commercial publishers).
- (b) Translated into other languages through National Adhering Organizations.

For Reports published earlier in 1973, see Bulletin No. 45 (May 1973), page 100.

APPENDICES TO IUPAC INFORMATION BULLETIN

The following Appendices were issued in August 1973:

Appendices on Tentative Nomenclature, Symbols, Units, and Standards

- No. 30 Classification and Nomenclature of Electroanalytical Techniques (Commission on Electroanalytical Chemistry)
- No. 31 Nomenclature of Organic Chemistry, Section D: Organic Compounds containing Elements which are not exclusively Carbon, Hydrogen, Oxygen, Nitrogen, Halogen, Sulfur, Selenium, and Tellurium (Commissions on Nomenclature of Organic and Inorganic Chemistry)
- No. 32 Nomenclature of Iron-Sulfur Proteins (IUPAC-IUB Commission on Biochemical Nomenclature)
- No. 33 Nomenclature and Conventions for Reporting Mössbauer Spectroscopic Data (Commission on Molecular Structure and Spectroscopy)

Technical Reports

- No. 7 A Survey of Some Recommended Methods for Identification and Determination of the Phenol Group (Commission on Analytical Reactions and Reagents)
- No. 8 Recommended Method for Aflatoxins in Cocoa Beans (Commission on Food Contaminants)

Subscribers to the *Information Bulletin* receive all Appendices automatically and free-of-charge on publication. Gratis copies may also be obtained by writing to:

Assistant Secretary (Publications)
IUPAC Secretariat
Bank Court Chambers
2-3 Pound Way
Cowley Centre
Oxford OX4 3YF, UK

For Appendices issued earlier, see *Information Bulletin* No. 45 (May 1973, page 97). Tentative Nomenclature Appendices Nos. 1-13, 20, 21, and 28 and Technical Reports Nos. 3-5 are now out of print.

Subject to the prior agreement of IUPAC, its tentative nomenclature recommendations may be:

- (a) Republished in other journals.
- (b) Translated into other languages through National Adhering Organizations.

CALENDAR OF IUPAC-SPONSORED MEETINGS

1974

January 14-18	V International Symposium on Magnetic Resonance (Prof. B. VENKATARAMAN, Chairman of Local Organizing Committee, V International Symposium on Magnetic Resonance, c/o Tata Institute of Fundamental Research, Homi Bhabha Road, Bombay 5, India)	Bombay (India)
March 24-29	IV International Conference on Crystal Growth (Conference Secretariat, Organizing Committee of ICCG-IV, Science Council of Japan, 7-22-34 Roppongi, Minato-ku, Tokyo 106, Japan)	Tokyo (Japan)
March 25-29	II International Meeting on Boron Chemistry (Prof. M. G. H. WALLBRIDGE, Secretary, II IME BORON, c/o Department of Molecular Sciences, University of Warwick, Coventry CV4 7AL, UK)	Leeds (UK)
April 29- May 2	II IUPAC Conference on Physical Organic Chemistry (Prof. TH. J. DE BOER, II IUPAC Conference on Physical Organic Chemistry, c/o Laboratorium voor Organische Scheikunde, Universiteit van Amsterdam, Nieuwe Achtergracht 129, Amsterdam, Netherlands)	Noordwijkerhout (Netherlands)
June 10-12	International Symposium on Laboratory Instruction in Chemistry (Prof. R. L. STRONG, Department of Chemistry, Rensselaer Polytechnic Institute, Troy, New York 12181, USA)	Troy/ New York (USA)
June 24-28	IX International Symposium on Chemistry of Natural Products (M. K. WARD, Executive Secretary, IX International Symposium on Chemistry of Natural Products, c/o National Research Council of Canada, Ottawa, Ontario K1A 0R6, Canada)	Ottawa (Canada)
July 3-9	III International Pesticide Chemistry Congress (Dr. J. LARINKARI, Chairman of Organizing Committee, III International Pesticide Chemistry Congress, POB 28, SF-00131 Helsinki 13, Finland)	Helsinki (Finland)
July 10-12	IV International Conference on Nonaqueous Solvents (Dr. H. SCHINDLBAUER, IV ICNAS, c/o Verein Österreichischer Chemiker, Eschenbachgasse 9, A-1010 Wien, Austria)	Vienna (Austria)
July 26-31	International Symposium on Macromolecules (Prof. E. B. MANO, Simpósio Internacional de Macromoléculas, c/o Academia Brasileira de Ciências, Caixa Postal 229, 20.000 Rio de Janeiro, GB, Brazil)	Rio de Janeiro (Brazil)
August 5-9	VII International Symposium on Carbohydrate Chemistry (Dr. S. BAUER, Chairman of Organizing Committee, VII International Symposium on Carbohydrate Chemistry, c/o Institute of Chemistry, Slovak Academy of Sciences, Dúbravská cesta, CS-809 33 Bratislava, Czechoslovakia)	Bratislava (Czechoslovakia)
August 19-24	XVI International Conference on Coordination Chemistry (Dr. W. J. DAVIS, Secretary of Organizing Committee, XVI-ICCC, c/o Department of Chemistry, Trinity College, University of Dublin, Dublin 2, Ireland)	Dublin (Ireland)
August 26-29	XIV Prague Microsymposium on Macromolecules: Crosslinking and Networks (PMM Secretariat, c/o Institute of Macromolecular Chemistry, Czechoslovak Academy of Sciences, Heyrovského náměstí 2, CS-162 02 Praha 6, Czechoslovakia)	Prague (Czechoslovakia)
August 26-30	I IUPAC Conference on Synthetic Organic Chemistry (Prof. A. BRUYLANTS, I IUPAC Conference on Synthetic Organic Chemistry, c/o Laboratoire de Chimie Générale et Organique, Université de Louvain, Naamsestraat 96, B-3000 Louvain, Belgium)	Louvain (Belgium)

August 26-31	IV Polish Conference on Analytical Chemistry (Dr. R. DYBCZYNSKI, Secretary of Organizing Committee, IV Polish Conference on Analytical Chemistry, c/o Institute of Nuclear Research, Dorodna 12, Warszawa, Poland)	Warsaw (Poland)
September 9-13	IV International Symposium on Medicinal Chemistry (Secretariat, IV International Symposium on Medicinal Chemistry, c/o Merck Sharp & Dohme NV, Professional & Government Liaison, Waarderweg 39, POB 581, Haalem, Netherlands)	Noordwijkerhout (Netherlands)
September 10-14	II Symposium on Inorganic Phosphorus Compounds (Secretariat, II Symposium on Inorganic Phosphorus Compounds, c/o Department of Inorganic Chemistry, Prague Institute of Chemical Technology, Suchbátarova 5, CS-166 28 Praha-Dejvice, Czechoslovakia)	Prague (Czechoslovakia)
September 15-20	International Symposium on Macromolecules (Prof. J. G. FATOU, General Secretary of International Symposium on Macromolecules, Instituto de Plásticos y Caucho, c/o Juan de la Cierva No. 3, Madrid 6, Spain)	Madrid (Spain)
September 23-27	II International Symposium on Chemistry of Non-benzenoid Aromatic Compounds (Dr. W. FRITSCH, General Secretary of Organizing Committee, II International Symposium on Chemistry of Nonbenzenoid Aromatic Compounds, c/o Gesellschaft Deutscher Chemiker, Postfach 119075, D-6000 Frankfurt/Main 8, German Federal Republic)	Lindau (German Federal Republic)
1975		
June 6-11	XXV IUPAC Congress (Organizing Committee, XXV IUPAC Congress, POB 16271, Tel Aviv, Israel)	Jerusalem (Israel)
August 25-29	IV International Symposium on Chemistry of Carotenoids other than Vitamin A (Dr. O. ISLER, F. Hoffmann-La Roche & Co. AG., Grenzacherstrasse 124, CH-4002 Basel, Switzerland)	Bern (Switzerland)
September	XXVIII IUPAC Conference: closed meeting of IUPAC bodies (Executive Secretary IUPAC, IUPAC Secretariat, Bank Court Chambers, 2-3 Pound Way, Cowley Centre, Oxford OX4 3YF, UK)	(Spain)
1976		
July 12-16	VI International Congress on Catalysis (Dr. D. A. WHAN, Secretary of Organizing Committee, VI International Congress on Catalysis, c/o Department of Chemistry, University of Edinburgh, West Mains Road, Edinburgh EH9 3JJ, UK)	London (UK)

ATOMIC WEIGHTS OF THE ELEMENTS: 1973

At the XXVII IUPAC Council meeting, held in Munich on 29 and 31 August 1973, the following changes in recommended values for atomic weights were approved:

Nickel from 58.7₁ to 58.70

Rhenium from 186.2 to 186.207

These changes together with important new annotations and listings will be in the full report of the Commission on Atomic Weights to be published early in 1974 in the IUPAC journal *Pure and Applied Chemistry*. This report will also contain the full Table of Atomic Weights 1973.

CALENDAR OF NON-IUPAC MEETINGS

1974

February 19-20	II International Conference on Carbon Fibres: Their Place in Modern Technology (Mr. D. H. COHEN, Assistant Secretary, Plastics Institute, 11 Hobart Place, London SW1W 0HL, UK)	London (UK)
March 25-27	International Conference on Plastics in Agriculture and Horticulture (Mr. C. A. BRIGHTON, BP Chemicals International Ltd., UK Plastics Department, Devonshire House, Piccadilly, London W1X 6AY, UK)	Ashford (UK)
April 1-5	Annual Chemical Congress of Chemical Society and Royal Institute of Chemistry (Dr. J. F. GIBSON, Chemical Society, Burlington House, Piccadilly, London W1V 0BN, UK)	London (UK)
April 18-24	International Conference on Excited States of Biological Molecules (Dr. J. B. BIRKS, Atomic, Molecular, and Polymer Physics Group, Department of Physics, Schuster Laboratory, University of Manchester, Manchester M13 9PL, UK)	Lisbon (Portugal)
May 16-18	VIII International Working and Discussion Meetings of International Association for Cereal Chemistry (Dr. F. SCHWEITZER, Secretary General ICC, Schmidgasse 3-7, A-2320 Schwechat, Austria)	Vienna (Austria)
May 28-31	III Symposium on Ion-exchange (Hungarian Chemical Society, POB 240, H-1368 Budapest, Hungary)	Balatonszéplak (Hungary)
June 2-5	LVII Annual Conference of Chemical Institute of Canada (Chemical Institute of Canada, Room 906, 151 Slater Street, Ottawa, Ontario K1P 5H3, Canada)	Saskatchewan (Canada)
July 1-5	VI International Symposium on Organo-Sulfur Chemistry (VI Organic Sulfur Symposium, School of Physical and Molecular Sciences, University College of North Wales, Bangor LL57 2UW, UK)	Bangor (UK)
September 22-25	International Symposium on Electro-optical Properties of Macromolecular Solutions (Dr. C. HOUSIER, Laboratoire de Chimie Physique, Université de Liège au Sart-Tilman, B-4000 Liège, Belgium)	Liège (Belgium)
September 22-27	IV International Congress of Food Science and Technology (Secretaría del IV Congreso Internacional de Ciencia y Tecnología de Alimentos, c/o Instituto de Agroquímica y Tecnología de Alimentos, Jaime Roig 11, Valencia-10, Spain)	Madrid (Spain)
December 2-6	XIX International Dairy Congress (Congress Secretariat, Vigyan Bhavan Annexe, Maulana Azad Marg, New Delhi 110 011, India)	New Delhi (India)

IUPAC COLLEAGUES DECEASED

We have been informed of the death of:

- Sweden* Dr. I. BOSUND (17 July 1973)—Applied Chemistry Division Committee (1971-)
Prof. H. LUNDIN (24 March 1973)—Section on Fermentation Industries (1957-1969)
- USA* Dr. C. N. FREY (27 September 1972)—Section on Fermentation Industries (1957-1965)

XXIV IUPAC CONGRESS

Hamburg, 2-8 September 1973

The scientific programme was held in the newly built Hamburg Congress Centre. In his opening remarks, Prof. F. LYNEN, Chairman of the Organizing Committee and President of Gesellschaft Deutscher Chemiker, dealt briefly with the world progress of chemistry during the 14 years since the last IUPAC Congress took place in Germany, at Munich in 1959.

The present Congress attempted to provide a survey of the present state of developments in a series of important fields of chemical science in 7



Prof. F. LYNEN (on left) talks to Prof. G. T. SEABORG (USA) at the plenary opening session, at which Prof. SEABORG delivered his plenary lecture on 'Status Report on the Trans-uranium Elements'

Sections and 2 Joint Symposia with 6 Plenary Lectures, 66 Main Sectional Lectures, and over 300 Discussion Lectures. In addition, numerous excursions gave participants information from everyday practice, and cultural and social events a framework for personal contact. There were about 1,500 registered participants from 36 different countries of the eastern and western hemispheres.

Rapid publication of the Plenary and Main Lectures (for details see Bulletin No. 45, May 1973, pages 74-78) from the 7 Sections:

- 1—High Polymers
- 2—Chemistry of Natural Products
- 3—Solid State Chemistry
- 4—Compounds of Non-metals
- 5—Applied Electrochemistry
- 6—Radiochemistry
- 7—Symposium on Information and Communication in Chemistry

is currently in progress by photooffset printing directly from manuscripts supplied by the lecturers at Munich. The 7 volumes are expected to be available from Messrs. Butterworths (London), official publisher of IUPAC, in December 1973.

The main lectures from the 2 Joint Symposia:

Medicinal Chemistry—Polypeptide Hormones and Releasing Factors

Modern Methods for Treatment of Waste Water in Theory and Practice will appear during 1974 in the IUPAC journal, *Pure and Applied Chemistry*.

LIST OF ABBREVIATIONS

CEE	Communauté Européenne Economique
COSPAR	ICSU Committee on Space Research
COWAR	ICSU Committee on Water Research
FAO	UN Food and Agriculture Organization
GARP	Global Atmospheric Research Programme
IARC	WHO International Agency for Research on Cancer
IBP	International Biological Programme
ICSU	International Council of Scientific Unions
IGU	International Geophysical Union
IUB	International Union of Biochemistry
IUBS	International Union of Biological Sciences
IUGG	International Union of Geodesy and Geophysics
IUGS	International Union of Geological Sciences
IUNS	International Union of Nutritional Sciences
IUPAB	International Union of Pure and Applied Biophysics
IUPAP	International Union of Pure and Applied Physics
IUPS	International Union of Physiological Sciences
IUTAM	International Union of Theoretical and Applied Mechanics
MAB	Man and the Biosphere Programme
NBS	US National Bureau of Standards
SCAR	ICSU Scientific Committee on Antarctic Research
SCIBP	ICSU Special Committee for the International Biological Programme
SCOR	ICSU Scientific Committee on Oceanic Research
SCOPE	ICSU Scientific Committee on Problems of the Environment
UN	United Nations
UNESCO	UN Educational, Scientific and Cultural Organization
WHM	World Meteorological Organization
WHO	UN World Health Organization

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**INTERNATIONAL UNION OF PURE
AND APPLIED CHEMISTRY**

**UNION INTERNATIONALE DE CHIMIE
PURE ET APPLIQUÉE**

**INFORMATION BULLETIN
NUMBER 47**

MARCH 1974

IUPAC SECRETARIAT

**Bank Court Chambers, 2/3 Pound Way
Cowley Centre, Oxford OX4 3YF, UK**

**Telephone—Oxford 770125 & 772834
Telegrams—IUPAC OXFORD**

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International Union of Pure and Applied Chemistry
1974**

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

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IUPAC INFORMATION BULLETIN

The Bulletin provides a news medium for the various activities of IUPAC, especially of its 40 or so committees which deal with chemical topics needing regulation, standardization or codification. It carries advance information on forthcoming symposia which are to be sponsored by IUPAC together with reports of such meetings which have recently taken place. Coverage is also given to projects in which IUPAC is collaborating with other international organizations.

Two series of Appendices to the Bulletin are issued:

- (i) Appendices on Provisional Nomenclature, Symbols, Units, and Standards
- (ii) Technical Reports

Bulletin No. 47 completes the issues under the 1973 subscription. In 1974 there will be two issues (Nos. 48 and 49). Annual subscription to the Bulletin, inclusive of the two series of Appendices and postal charges, is US \$9.00 or £3.00 (surface); US \$18.00 or £6.00 (Bulletin and Appendices by air); US \$15.00 or £5.00 (Bulletin by surface and Appendices by air); US \$12.00 or £4.00 (Bulletin by air and Appendices by surface).

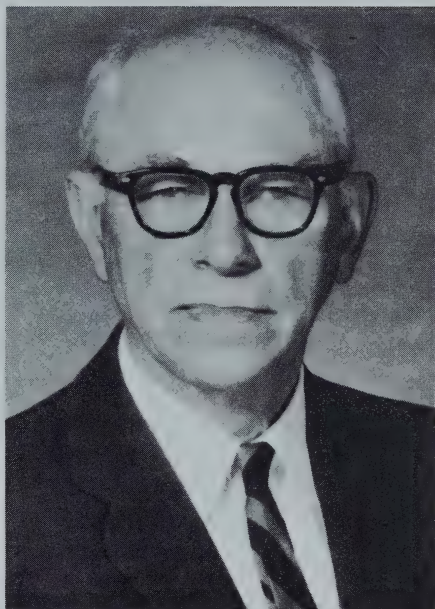
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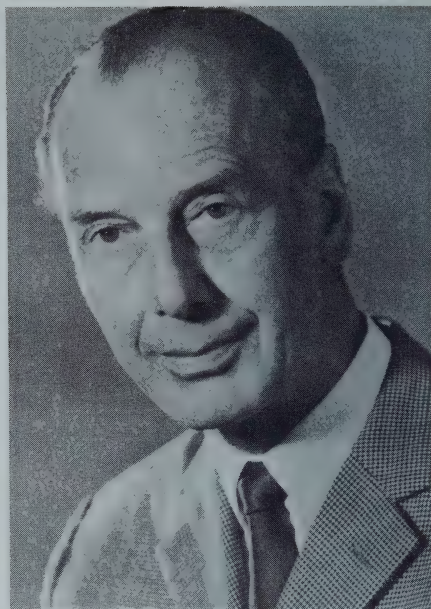
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1967-1969



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1969-1973



Prof V Gutmann Austria

1973-1977

REPORTS OF IUPAC BODIES

IUPAC-IUB COMMISSION ON BIOCHEMICAL NOMENCLATURE (CBN)

Meersburg, 20-23 June 1973

Present: Prof. O. HOFFMANN-OSTENHOF (Chairman), Dr. W. E. COHN (Secretary), Prof. A. E. BRAUNSTEIN, Dr. B. L. HORECKER, Prof. P. KARLSON, Dr. B. KEIL, Prof. C. LIÉBECQ, Prof. E. C. WEBB, Prof. W. J. WHELAN. Dr. K. L. LOENING participated as an Observer from the Commissions on Macromolecular Nomenclature (CMN) and on Nomenclature of Organic Chemistry (CNOC) and Dr. R. DYBKAER as an Observer from the Commission on Quantities and Units in Clinical Chemistry (CQUCC).

Enzyme Nomenclature, Recommendations 1972

Since the last meeting of CBN (see *Information Bulletin* Nos. 42/43, July 1972, pp. 11-12), the Enzyme Book had been published by Elsevier. CBN visualized periodical supplements to or revisions of the Enzyme Book. To make this as effective and complete as possible, CBN wished to invite anyone who discovered an enzyme activity not now in the book, or who had a criticism of any material in the book, to communicate the same to WEBB, either directly or through CBN. WEBB, assisted by JAKOBY and KELETI, would constitute CBN's Supplement Subcommittee. CBN would ask the IUB Commission of Editors of Biochemical Journals (CEBJ) and other avenues of publicity to publish a call for such information, preferably in the form used in the Enzyme Book or as reprints, to be submitted. CBN Members were asked to be on the alert for the appearance of papers describing new activities, and editors would be asked to do likewise.

Abbreviations and Symbols, 1965

Sections 2 and 5 were essentially replaced by the Peptide and Nucleic Acid documents of 1972 and 1970, respectively. Section 3 might be replaced by a separate document constructed in collaboration with the Carbohydrate Subcommittee (see later). Section 4 might be replaced by the Biochemical Organophosphorus document (see later). Nevertheless, a brief exposé of the fundamentals of each of these Sections in a single document was desired by editors. The Subcommittee (DILLMANN, KLYNE, and COHN) was to be activated by asking DILLMANN to prepare a first draft.

Miscellaneous Compounds ('Vitamins')

CBN would explore the possibility of a joint document with IUNS, to resolve minor formal differences, but saw no substantive revisions necessary at the moment.

Folic Acids

This document should be revised to accord formally with IUNS. COHN was to undertake this revision.

Quinones with Isoprenoid Side Chains

This document had been revised and was ready for approval and publication

as soon as (a) a stereochemical note, proposed by LOENING, and (b) examples of dihydro and other modified forms, were included.

Lipid Proposals

This document should be revised, largely by expansion of its Section 2, and should include, or accord with, the lipid part of the glycolipid work (see later). Part 1 (the *sn* system) had been widely accepted. KARLSON would act as convenor.

Cyclitols

This joint document with CNOC had been submitted for Union approvals by the Chairman prior to publication.

Steroids

This joint document with CNOC had been published in definitive form during 1972. KLYNE would be asked to act as the collector of corrections or suggestions for revision.

Vitamins B-6 (1972 Revision)

These recommendations had appeared in *Pure and Applied Chemistry*. However, the revisions made, in the advancement of this document for IUPAC from tentative to definitive version, were too numerous to make practical the publication, by CEBJ, of a list of changes. Therefore, a Revised Recommendation (1973) was to be prepared by COHN for CEBJ.

Polypeptide Conformations

The Chairman would ask KENDREW if any revisions appeared necessary.

Carbohydrates—I

The objections raised by the Anglo-American committees during the formulation of the tentative document published with CNOC had not been restated or reintroduced. Because these were considered earlier and because no others had been raised, CBN saw no need to revise the present document and would so inform CNOC.

Multiple Forms of Enzymes

The one objection received was considered during formulation. No action was proposed.

Tetrapyrroles

A third memorandum from BONNETT (convenor of the CNOC-CBN Subcommittee) had been received. CBN agreed with the principle therein of dropping the Fischer system and numbering in the manner of corrin. CBN also agreed to the α , β system of stereochemical designation and had adopted this in its corrinoid documents. There were still questions concerning the 'linear' compounds to be resolved.

Carbohydrates—II et seq.

Conformations of Monosaccharides, approved by the Anglo-American committees (HORTON and OVEREND, Chairmen) and intended for early publica-

tion by them in *J. Chem. Documentation*, had been circulated to CBN and CEBJ and was under active consideration by the CNOC-CBN Subcommittee on Carbohydrate Nomenclature (WHELAN, convenor).

Unsaturated Carbohydrates was not yet approved by the Anglo-American committees; it had been sent to CBN and to the CNOC-CBN Subcommittee.

Polysaccharide Nomenclature, based on the 'glycan' principle, was similarly not yet approved by the Anglo-American committees. It had been distributed in similar fashion. It had been criticized (COHN and TIPSON) as (i) being too definite about indefinite structures, (ii) being incompatible with symbolic representations, and (iii) failing to utilize the principles of CBN's systems for symbolizing polynucleotides and polypeptides. CBN proposed an *ad hoc* Subcommittee (COHN and FOX, with advice from WHELAN and HORECKER) to prepare alternatives to those parts of the document that seemed presently ambiguous or that could be handled adequately by the present system (of 'poly' prefix or 'n' suffix).

Peptidoglycans

The first draft document received from JEANLOZ (and distributed to CBN) was considered. CBN decided to differentiate peptidoglycans from glycoproteins on the basis of the main chain. The former clearly should be integrated with the carbohydrate work, as should the carbohydrate portions of the latter. JEANLOZ would be asked to join the CNOC-CBN Subcommittee on Carbohydrate Nomenclature, which was concerned with these matters.

Conformation

Polysaccharides. MARCHESSAULT (convenor) had promised a report after a meeting in July.

Polynucleotides. CRAMER (convenor) had sent in, as a report, a reprint entitled 'Conformation of Biological Molecules and Polymers' from *The Jerusalem Symposia on Quantum Chemistry and Biochemistry, V, 1973*. This article summarized tentative proposals on this subject by some members of an *ad hoc* group of experts chaired by SUNDARALINGAM. CBN would study this document.

General. CBN had received a request from SCHERAGA, Chairman of an IUPAB committee concerned with these matters, to join with CBN in its conformation work. This possibility would be explored.

Amino-acid Nomenclature

This document had been approved in principle by CBN and by CNOC. CBN agreed to a modified numbering system for the alicyclic amino acids, in which the cyclic portions would receive unprimed numbers according to the basic ring systems involved, while the aliphatic portions would receive Greek-letter locants according to the classical system (α =amino carbon). This would resolve the histidine-histamine and the tryptophan-tryptamine problems. It was hoped that CNOC, which was now reviewing the document, would see to the proper names in the Appendix. Structural formulae should be included for more of the entries. It was agreed that 'residue' should be used for all units lacking an amino hydrogen atom and that 'cystyl' should be added.

Peptide Hormones

CBN should check the proposed names for possible duplication of trade-marked (registered) names; however, USAN or INN names need not be avoided. The individual names proposed were reviewed and many were altered. Etymological purity was preferred to brevity. Abbreviations for species names would not be included. KARLSON would prepare a new document for CBN, CEBJ, and expert advisors.

Cytochromes

An expert Subcommittee convened by KAMEN would meet shortly to consider this subject.

Corrinoid Nomenclature and Symbolism

CNOC had been consulted with respect to the first two documents and IUPAC Commission on Nomenclature of Inorganic Chemistry (FERNELIUS) would be consulted. Barring serious objections, these documents were finished. CBN decided to publish the two as a single document, with Symbolism as an appendix to Nomenclature.

Tocopherols

The tortuous history of this document and the many discussions with IUNS were reviewed. For legal reasons, particularly in USA, it appeared necessary to avoid the prefix *nat* (for 'natural'). *RRR* seemed proper. CBN wished to deemphasize *d* and *l* and to urge that names using these prefixes be cross referenced to recommended names. Further consultations with the nutritionists would be necessary in view of the changes required or recommended. HOFFMANN-OSTENHOF would then prepare a revised draft.

Non-Enzyme Proteins

CBN was considering many classes of these, *e.g.*, haemoglobins, caseins, histones, fibrinogens, and blood-clotting proteins, glycoproteins, toxins, globulins, contractile proteins, *etc.*, with the first four of these taking first priority. KEIL was the convenor for the general subject and would suggest specific subgroups for each. One of these would be on histones, and BONNER was proposed as convenor.

Interconvertible Enzymes

A preliminary draft of proposals by an *ad hoc* Subcommittee headed by HOLZER was distributed by HORECKER and discussed. Modifications suggested by CBN would be referred back to the Subcommittee.

Phosphorus Compounds of Biological Importance

A preliminary draft document prepared by COHN with advice from HOFFMANN-OSTENHOF and KLYNE was distributed and discussed. CBN members were to suggest changes, additions, and deletions, both as to general principles and to individual entries in the tables, to COHN, who would prepare a revised document after consulting CNOC's Section D-Rules, now in press with IUPAC.

Isotopically Modified Compounds

A draft document, prepared by the American Chemical Society's Organic

Nomenclature Committee, had been presented to CNOC for consideration. COHN and LOENING (both members of the ACS Nomenclature Committee) discussed the features of this proposal, which endorsed the CEBJ/ACS-CS system for 'labelled' compounds and the Boughton system for 'substituted' compounds (or molecules), together with definitions of these terms not heretofore made. The Chairman would express CBN's general and specific interests in this document to CNOC.

Prostaglandin Nomenclature

Two proposals and a counter-proposal, made originally to the ACS Nomenclature Committee, had become known to CBN. Although logically a part of the natural products area now being worked out by CNOC, it was decided that copies of the basic material should be distributed to all CBN Members in order that they might ascertain the degree and depth of interest of CBN in this subject. KARLSON would convene a Subcommittee to advise on the matter.

Immobilized Enzymes

A document drafted by an *ad hoc* Subcommittee in 1971 had been received by CBN. CBN discussed the proposals made in this document as well as some counter-proposals. COHN would communicate CBN's thoughts to the originators of the proposals.

Catecholamines

HORECKER would consult UDENFRIEND as to the need for any CBN action in this area.

Glycosphingolipids

WIEGANDT joined CBN to summarize the present status of the work of his Subcommittee in this area. The oligosaccharide part would be integrated with the CNOC-CBN oligosaccharide document and the lipid part with the revision of lipids (see earlier). CBN discussed various approaches to the problem and made several suggestions to the Subcommittee.

Nomenclature of the Chains of Serine Proteinases

KEIL had prepared a draft document, which would be sent to CBN and to an *ad hoc* Subcommittee for criticism.

Cooperation with CNOC

The distribution to Members of CBN and CNOC of a fourth draft of a natural products document was noted. KLYNE being absent, the Chairman read a letter from him summarizing a meeting with LOZAC'H on all matters currently concerning CBN and CNOC. CNOC expected CBN to originate documents dealing with specific areas of biochemical interest, CNOC's role being to ensure maximum agreement with the general rules of organic chemistry. CNOC had examined all current CBN and CBN-CNOC documents now in final or near-final stages; there appeared to be no significant disagreements.

Cooperation with CMN

LOENING described present activities of CMN on (a) definitions, (b) copolymers, (c) stereochemical designations, (d) inorganic polymers. Item (c)

concerned CBN and collaboration was desirable. CBN expressed its need for advice from CMN in the matter of abbreviations for source-based names, an area that CMN had not entered but in which CBN had to act. Assistance was also required in connection with polysaccharide nomenclature (see earlier).

Relations with CEBJ

(a) CBN considered it very important to have a Member, preferably an Officer, of CEBJ to meet with it, either as a Member (as at present) or as an Observer. (b) CBN considered it important to meet jointly with CEBJ every two or three years, and planned to do so again in 1975.

Cooperation with CQUCC

DYBKAER asked for some advice on behalf of CQUCC. It was agreed that the new important derived kind of quantity in enzymology was named *enzymic activity* by CBN; its derived coherent SI unit was mol/s, which CBN called katal; its symbol was not stated by CBN, but the suggestion *z* was accepted. The correct CBN names for two other derived kinds of quantity were *specific enzymic activity* (unit: mol/(s kg) or kat/kg) and *molar enzymic activity* (unit: s⁻¹ or kat/mol). It was agreed that the derived kind of quantity name *concentration of enzymic activity* (unit: mol/(s l) or kat/l) was cumbersome, but it was feared that 'enzymic concentration' might be misunderstood for 'substance concentration of enzyme protein'. A suggestion for a better name would be considered as would symbols for these three kinds of quantity.

W. E. COHN

COMMISSION ON NOMENCLATURE OF ORGANIC CHEMISTRY (CNOC)

Würzburg, 15-22 August 1973

Present: Prof. N. LOZAC'H (Chairman), Mr. S. P. KLESNEY (Secretary), Dr. K. BLÁHA, Dr. L. C. CROSS, Dr. K. L. LOENING, Prof. J. RIGAUDY, Prof. S. VEIBEL (Titular Members); Dr. H. GRÜNEWALD, Dr. K. HIRAYAMA, Prof. F. VÖGTLE (Associate Members); Prof. O. HOFFMANN-OSTENHOF [Observer from IUPAC-IUB Commission on Biochemical Nomenclature (CBN)]; Dr. D. M. P. MINGOS [Observer from Commission on Nomenclature of Inorganic Chemistry (CNIC)].

Reorganization of IUPAC Nomenclature Work

The following scheme was proposed and discussed. In the first stage only governing principles should be discussed and adopted. They should be brought to the attention of editors of chemical publications through the agency of special advance information notes. In this way, editors would be informed at an early stage of the general trend of the recommendations-to-be, avoiding excessive disagreements between the nomenclature effectively used in papers.

Advance information notes were mainly usable by people having already a good knowledge of the principles of nomenclature. In a second stage it

would be necessary to produce more detailed recommendations, taking advantage of the opinions expressed by those who used the advance information notes.

Phane nomenclature and nomenclature of natural products (see later) were two areas where the scheme might be tested. Emphasis would be on speed of publication, not on perfection of the proposals at that stage.

Isotopically Modified Compounds

A project group composed of RIGAUDY (convenor), MINGOS, and KLESNEY, prepared a document on isotopically modified compounds, which was reviewed by CNOC. RIGAUDY would incorporate the agreed changes into a new document which would be distributed to CNOC and to the Officers of CNIC and CBN.

Cyclophanes and Polycyclic Arrays of Carbon Atoms

The nomenclature of cyclophanes of HIRAYAMA was discussed and its principles approved. It appeared that a more systematic treatment of polycyclic arrays of carbon atoms was highly desirable. LOZAC'H proposed an extension and revision of certain existing IUPAC rules, the general principles were approved, and he agreed to prepare a revised document. A project group on polycyclic arrays and cyclophanes was appointed, comprising LOZAC'H (convenor), HIRAYAMA, LOENING, and VÖGTLE. It was decided to ask KAUFFMANN and ECKROTH to participate in this work. Preliminary documents were prepared by the project group and discussed by CNOC. Revised documents would be distributed to CNOC when available.

Revision of Sections A, B, C, and D*

It was agreed that this work should be accomplished in close cooperation with Chemical Abstracts Service, whose document on 'Naming and Indexing of Chemical Substances (1972-1976)' should be carefully checked and compared with existing IUPAC rules in order to bring these rules and CAS recommendations in as close agreement as possible. It was also decided to study particularly the nomenclature of carbocations.

A project group was established with GRÜNEWALD (convenor), CROSS, and LOENING as members. RIGAUDY would help in the field of carbocations, with which work TRAYNHAM would also be invited to participate.

Section E: Fundamental Stereochemistry

A project group consisting of KLYNE and CROSS (convenors), BLÁHA, GRÜNEWALD, and VEIBEL, was appointed to finalize Section E ready for publication in *Pure and Applied Chemistry*. A future extension of Section E was foreseen.

Natural Products

General Rules for Natural Products and Their Derivatives. The revised draft rules were to be extended by further examples and explorations so that they could stand independently of the existing type of appendix. This nomenclature was to be considered as Section F of *Nomenclature of Organic Chem-*

**Nomenclature of Organic Chemistry*, 1971 (combined Sections A, B and C); Section D: Tentative Nomenclature Appendix No. 31 to *IUPAC Information Bulletin*, August 1973.

istry. CROSS would prepare a further revised draft, which should be virtually read for publication as provisional recommendations.

Corrinoids. The CBN nomenclature document was approved by CNOC, subject to slight amendment, as a provisional document. HOFFMANN-OSTENHOF noted the objections of CNOC to the CBN document on symbolism for corrinoids, which was otherwise approved by CNOC as a provisional document.

Tetrapyrroles. CBN is continuing work on this document, which should also be sent to CNIC.

Indole Alkaloids. These compounds would be covered in the section on natural products. KLESNEY would send the present document to the Officers of CBN.

Carbohydrates. Three documents were discussed with HOFFMANN-OSTENHOF: 'Conformation of Monosaccharides' was considered as satisfactory; 'Unsaturated Monosaccharides' was generally acceptable but a few problems remained; for 'Polysaccharide Nomenclature' it was recommended that CBN should prepare a new set of rules. When these and several other pending documents on carbohydrate nomenclature were available, IUPAC should sponsor a meeting of the various groups involved, probably in 1974.

Cyclitols. The final document was being processed for publication in *Pure and Applied Chemistry*.

Lignins. A project group was proposed, consisting of CROSS (convenor), LOENING, NIMZ, SARKANEN, CBN representative.

Carotenoids. The published IUPAC provisional version was reconfirmed by CNOC as being acceptable as final recommendations.

Tocopherols. Comments were made by CNOC on the document prepared by CBN.

Quinones with Isoprenoid Side Chains. Subject to minor amendment, these rules were approved for final publication in *Pure and Applied Chemistry*.

Prostaglandins. A project group was being organized to deal with this subject, with KARLSON of CBN as convenor.

Amino Acids. BLÁHA and LOENING were asked to communicate their views to CBN on this document, which was otherwise approved by CNOC for publication.

Lipids. The cooperation of CNOC was requested for the revision of a document on lipids elaborated originally by CBN only. A project group was proposed of KARLSON (convenor), VEIBEL, and VÖGTLE.

Brazilin, Cannabinoids, Diterpenes. Brief consideration was given to nomenclature for these fields.

Membership

VEIBEL had completed his term as Titular Member, but should continue as an Associate Member. GRÜNEWALD was nominated to fill the vacancy of Titular Member.

Next Meeting

This was decided to be in UK during July or August of 1974.

N. LOZAC'H

MACROMOLECULAR DIVISION WORKING PARTY ON STRUCTURE AND PROPERTIES OF COMMERCIAL POLYMERS

Netherley, 7-8 September 1973

Present: Dr. A. J. DE VRIES (Chairman), Dr. M. CARREGA (Secretary), Dr. J. W. BARRETT, Dr. A. C. BASKETT, Dr. A. R. BERENS, Dr. J. CHAUFFOUREAUX, Mr. S. D. EAGLETON, Dr. J. HEIJBOER, Dr. T. T. JONES, Dr. J. MEISSNER, Dr. H. H. MEYER, Prof. G. PEZZIN, Dr. A. PLOCHOCKI, Dr. A. K. VAN DER VEGT, Mr. J. L. S. WALES, Dr. J. ZELINGER.

Meeting held at Frankfurt/Main (26-27 February 1973)*

The paper on elasticity of HDPE melts had not yet been received from FLEISSNER.

Orientation in Polystyrene Programme

JONES presented the final report on the effect of molecular orientation on the mechanical properties of PS. As to the glass transition temperature T_g , DE VRIES reported that Rhône-Progil had determined the T_g of the two PS by means of DSC and found 91 and 98 °C, which confirmed the difference between the two samples obtained by mechanical damping measurements.

The interpretation of the maximum shrinkage stress with the aid of the rubber elasticity theory was discussed extensively. Several Members were of the opinion that this part of the text might be developed somewhat more explicitly; in particular, it was suggested to give the complete Flory's formula taking account of the number of chain-ends. MEISSNER proposed to include a reference to the work by STÖLTING and MÜLLER [*Koll. Zeitschrift* **238**, 459 and **240**, 792 (1970)] concerning the relative importance of entropic and Hookean-elastic deformations in the case of oriented PS, determined by means of calorimetric measurements. Because environmental stress cracking had only been measured by one participant (BASF) using a particular method, it was decided that details and full reference should be given as done in Part 5 of the interim report.

The Chairman thanked JONES for his excellent synthesis of the numerous results obtained in this programme. It was decided to present this report at the Aberdeen Symposium (see pp. 29-30) and to pass to DE VRIES the slightly modified version for publication in *Pure and Applied Chemistry*.

Future Programme. A new programme on the relationship between structure and mechanical properties of oriented and nonoriented two-phase polymers, proposed by RETTING and ZELINGER, was accepted by the Working Party after some discussion. Although a programme on ABS polymers would have been preferred by several Members, it was agreed that a programme limited in time (about two years) and only concerned with rubber modified PS might constitute an appropriate transition between the programme on PS just finished and a future programme on ABS.

All Members had received the written proposal by RETTING and ZELINGER. Those willing to participate were invited to write to them before 1 November 1973 and specify:

*See *Information Bulletin* No. 45, May 1973, pp. 56-58.

- the kind of test they were willing to carry out
- the number and shape of specimens they would need

The overall plan would be prepared by RETTING and ZELINGER and sent to the participants before 1 February 1974.

PVC Rheology Programme

WALES presented his draft report issued on 22 August 1973. Some modifications were proposed:

- on p. 4, Table No. 8 L/R range: 36 to 120 in place of 40 to 120
- on p. 7, MEISSNER asked to suppress completely the paragraph giving the results of BASF; these results were considered not to be reliable because of the apparatus used

DE VRIES asked whether the analysis of the Pressure vs. L/R plots in terms of a pressure dependent viscosity could be made on the data of a larger number of laboratories. In order to enable WALES to try such an enlarged analysis, all participants were required to send the necessary numerical data to him before 1 November 1973. Also, DE VRIES pointed out that the effect of hydrostatic pressure could be deduced from the pressure data without any assumption on the mathematical form of the pressure dependence by means of a method described by CHOI and NAKAJIMA [*Proc. 5th Int. Congr. Rheol.*, Vol. 4, pp. 287-293 (1970)].

BERENS regretted that the thermal history of the PVC compound was not known: CHAUFFOUREAUX replied that Solvay could specify the extrusion conditions.

In order to complete cone-and-plate and dynamic measurements at lower temperatures than 200°C, it was agreed that it would be useful to have results obtained with the Rheometrics parallel plate viscometer. CHAUFFOUREAUX would try to obtain such data.

In order to elucidate the problem of a possible transition from particle to molecular flow, more data at 170 and 175°C would be required. Participating Members having data available at these temperatures were invited to send them to WALES, if they had not already done so.

More data (in tabular form) on die-swell obtained with capillaries of different diameter would also be welcome. The higher values for die-swell reported by BASF might be explained, according to MEISSNER, by the effect of annealing.

All new results had to be sent to WALES before the end of the year. A first draft of the final report on this programme was hoped to be ready for discussion at the next meeting early in 1974. The final version would be discussed at a meeting later in 1974, and, if possible, presented at the IUPAC Symposium on Macromolecules in Madrid (15-20 September 1974).

LDPE Rheology Programme

Interim Report, Part II, Item 3.4. The written comments of WALES on this report were discussed. Because it appeared difficult to reach complete agreement between MEISSNER and WALES during the meeting on certain specific points (correlation between optical and mechanical measurements), which were not directly relevant to the main objective of the programme: finding differences between samples A, B, and C, it was decided finally that this particular topic would be published separately in the form of a scientific paper by MEISSNER and WALES, who were free to choose the most appropriate journal for such a publication.

Final Report, Part I. This report, written by MEISSNER and corrected by LODGE, was now ready for publication. A proposal of MEISSNER to publish it together with Part II/1 was accepted. PLOCHOCKI drew attention to the following corrections to be made:

- Table 8: kgf/cm² instead of kg/cm²
- page 11: at the end of line 2: B instead of C

Also, PLOCHOCKI asked to include in footnote 1 on page 4, a statement that it had been confirmed by other participants (in particular IV and V) that differences between the samples appeared if the melt flow index was measured at lower temperatures (125 or 150°C). The significance of these results could possibly be discussed in a later section of the report (Elastic effects in extrusion flow).

Final Report, Part II/1. A first draft of this part, to be published together with Part I, was presented by MEISSNER. After some discussion the following modifications were agreed upon:

- the term 'stressing viscosity', introduced on page 5 with reference to Giesekus's definition, had to be replaced by another more appropriate term. Several Members proposed 'transient viscosity', but MEISSNER considered that a still better term had to be found. All Members were invited to send their suggestions and proposals to MEISSNER as soon as possible.
- the results of the dynamic measurements, given in the third column of Table C1—V were only preliminary results, according to DE VRIES and should not be included in the final report. Only the data in the next column obtained with another improved version of the Balance Rheometer, should be taken into account. It appeared then, that the three sets of data obtained with two instruments, were in rather good agreement also at low frequency.

The corresponding text on pages 10 and 11 had, therefore, to be modified. DE VRIES agreed to rewrite this section of the report; it was decided to suppress Table C1—V but to maintain Figure C1—IV after correction.

It was hoped that a first draft of the final Part (C3, C4, and C5) would be available to all participating Members four weeks before the next meeting. Possibly the whole report might be presented by MEISSNER at the IUPAC Symposium in Madrid (September 1974).

Mechanical Properties of PVC

Several Members had made known the kind of experiments they were intending to perform in the new programme on 'Tensile properties of rigid PVC', described in the letter by CHAUFFOUREAUX of 26 April 1973. The detailed programme and overall plan would be sent with the samples to all participating Members by CHAUFFOUREAUX before the end of October. Contributions to different parts of the programme had been promised by:

- Solvay
- ICI
- TNO
- BASF
- Montedison
- Rhône-Progil
- Technical University Prague

PEZZIN would probably also take part in this programme. The participation of GOODRICH (high speed tensile measurements) was still to be confirmed by COLLINS. The proposal of ICI to enlarge the programme by including the effect of extrusion output rate would be discussed between CHAUFFOUREAUX and VINCENT, but it was generally agreed that the influence of processing variables on the mechanical properties of PVC, because of its great technological interest, might be better investigated in a new programme of which ICI could be coordinator.

For the samples to be investigated in the present programme, Solvay was requested to supply all relevant information, in particular: the conditions of extrusion and specimen preparation (date, annealing temperature, cooling rate, etc.).

In reply to a proposal by AJROLDI it was decided that in the second part of the programme, concerned with the effect of structure defects caused by presence of fillers, other test pieces than those defined by ISO R 527, type I might be used by the participants who would prepare their specimens from the sheets supplied by Solvay.

Structure and Properties of Block Copolymers

VAN DER VEGT gave a summary of the actual state of knowledge about the structure and properties of tri-block copolymers, in particular the Polystyrene-Polybutadiene-Polystyrene copolymers manufactured by Shell. Both melt and solid state properties were complex, time dependent, and strongly influenced by thermomechanical history. The anisotropy of the mechanical behaviour was due to morphological orientation (formation of domains) which, in contrast to molecular orientation, might be favoured by annealing at high temperature.

Melt viscosity was much higher than for the corresponding homopolymers. The molecular structure of these copolymers was simple and well defined although commercial products might contain small quantities of homo- and diblock-copolymer.

Because of its particular structure and properties on the one hand, and because its industrial importance was expected to grow rapidly on the other hand, this type of copolymer might present an interesting object of investigation for the Working Party. MEYER had already presented a written proposal for a programme on melt rheology of block copolymers which might serve as a starting point for a more extended programme.

VAN DER VEGT was invited to send a definite proposal to all Members before the end of the year. One or two commercial SBS-copolymers could be supplied by Shell, having the following characteristics:

PS-content	M of PS-blocks	M of PB-block
30%	14,000	64,000
22%	9,500	67,000

The inclusion of the latest commercial copolymer of Shell (Kraton G) in which the central block had been hydrogenated, might also be envisaged.

Because the thermal history and other experimental conditions might strongly affect the results of rheological measurements, MEISSNER proposed to start the programme with one polymer in order to study first the influence of various experimental parameters. The interest of optical measurements (light scattering?) during shearing or on a sheared sample after quenching was also mentioned.

The definitive proposal by VAN DER VEGT for a programme, that would have to take into account the available amount of material to be supplied by Shell, would be discussed in all its details at the next meeting.

Tentative Rules for the Working Party

The list of tentative rules distributed to all Members with the Minutes of the previous Meeting, were discussed. In reply to a question by MEISSNER concerning Rule 1, it was specified that each person was a Member as an individual representing a laboratory. As proposed by MEISSNER, the following words were added to Rule 3: 'except by special request from a member laboratory'. Rule 6 was completed as follows:

'An abstract of each Final Report will be prepared by the author(s) for publication in national and international journals in the field of polymers and plastics. In the Abstract full reference will be given to the published Final Report.'

Publications

In accordance with the extended Rule 6, CHAUFFOUREAUX was asked to prepare an Abstract of the Final Report on the Mechanical Properties of PVC programme, which would shortly be published in *Pure and Applied Chemistry*. DE VRIES would then ask the Secretariat to take care of the distribution to various polymer journals.

JONES was requested to prepare the manuscript of the Final Report on the Orientation in Polystyrene programme, which was to be submitted for publication in *Pure and Applied Chemistry*.

DE VRIES would write to the organizers of the IUPAC Symposium in Madrid, asking them to reserve a special session for the presentation of two reports from the Working Party (LDPE-rheology and PVC-rheology).

Date and place of Next Meeting

The next meeting would be held in Brussels on 21-22 February 1974, at the kind invitation of Solvay.

M. CARREGA

COMMITTEE ON TEACHING OF CHEMISTRY

Wrocław, 22-23 September 1973

Present: Prof. R. W. PARRY (Chairman), Mr. D. G. CHISMAN (Secretary), Prof. J. A. CAMPBELL, Prof. C. N. R. RAO, Dr. P. SYKES (Members); Prof. A. H. GUERRERO, Prof. E. GIESBRECHT, Prof. E. RANCKE-MADSEN, Prof. M. LAFITTE, Prof. I. PAIS, Prof. G. ILLUMINATI, Dr. D. P. DEN OS, Prof. B. JEZOWSKA-TREZBIATOWSKA, Dr. M. D. ROBINSON, Prof. W. B. COOK (National Representatives). A number of Observers were present, including representatives of UNESCO and the Federation of European Chemical Societies (FECS).

Minutes of Meeting in Washington, DC (19-20 July 1971)

The minutes of the previous meeting (*Comptes Rendus XXVI Conference*, pp. 76-80) were approved. Arising from the minutes, it was agreed to ask

the Secretariat to prepare a list of publications sponsored by the Committee or produced by the Committee in conjunction with UNESCO, for distribution to National Representatives and others interested in chemical education.

Membership

The Chairman reported that two of the Foundation Members—Prof. M. OKI and Prof. G. M. SCHWAB—had completed their terms of office. Proposals for possible replacements had been submitted to the President and the Executive Committee. It was noted that the South African National Committee for IUPAC had nominated Prof. R. R. ARNDT to replace Prof. C. J. H. SCHUTTE as its National Representative.

Advisory Comments on UNESCO Programme 1975-76

The Committee considered the draft recommendations of the International Congress on Improvement of Chemical Education (see pp. 33-37), particularly those directed at international organizations (Section 1), and came to the following conclusions, which they wished to submit to UNESCO as a guide to the formulation of the UNESCO programme in chemical education 1975-76.

Recommendation 1.1.1. The Committee endorsed the suggestion of major review conferences every four or five years and the idea of a report or a meeting to assess progress in implementing the recommendations of the 1973 Congress in two or three years' time.

Recommendation 1.1.2. The Committee endorsed the suggestion of regional meetings on scientific aspects of chemical education and recommended that one such meeting might be arranged as a small symposium at the time of the XXVIII IUPAC Conference in Spain (1975). Also, it recommended that the report of the Symposium on Educational Technology in Relation to Science Education, organized by UNESCO and ICSU in September 1972 in Paris and due to be published shortly in the UNESCO New Trends series, should be distributed to Members and to National Representatives.

Recommendation 1.2.1. The Committee considered that a panel on examinations (1.2.1.1) should be established, initially on a trial basis, using the knowledge and securing the cooperation of National Representatives. If successful, additional panels might be established.

Recommendations 1.3.1. and 1.3.2. These executive suggestions were mainly of direct concern to UNESCO, but were worthy of strong support.

Recommendation 1.3.3. The Committee endorsed this suggestion (see also *Newsletter* below).

Recommendation 1.4. The Committee endorsed all these suggestions for surveys and investigations, but considered that some would best be directed initially at national organizations rather than international ones (for instance 1.4.1 and 1.4.4). They expressed particular interest in the study of the relationship between brain function and national factors (1.4.4) and in the proposed survey on chemical education at tertiary level in Europe (1.4.10—see also *Laboratory Instruction Conference* below).

Recommendation 1.5. The Committee endorsed these suggestions for publications but considered that initially an international chemical education newsletter should be launched before an international journal (Recommendation 1.5.5, but see also under *Newsletter* below and Recommendation 1.3.3). It would, however, welcome further discussions with UNESCO on the question of an international journal.

Also, the Committee considered that a report on educational technology in the teaching of chemistry (Recommendation 1.5.3) might be based on the follow up of the UNESCO/ICSU Symposium on Educational Technology (September 1972), and might represent the proceedings of the symposium suggested for 1975 at the XXVIII IUPAC Conference in Spain. *Recommendations 1.6 and 1.7.* The Committee considered these innovative recommendations worthy of support but recognized that they had longterm relevance rather than immediate reference.

Tertiary Level Chemical Education in Europe

The Committee discussed the proposals of FECS for a survey of tertiary level chemical education in Europe, which was introduced by Prof. M. FRAZER, Dr. DEN OS, and Dr. P. FARAGO. It expressed interest in the proposal but explained to the representatives of FECS that IUPAC would not be in a position to help financially. Also, it expressed a wish to receive further details of the proposal and to be kept informed of developments. It was noted that the proposal was among the recommendations of the International Congress on Chemical Education (Recommendation 1.4.10) and that the UNESCO Division of Higher Education might be interested in collaboration or support.

Review of Committee Activities: 1964-1973

The Committee received a memorandum prepared by the Secretary, reviewing the activities of the Committee since its formation in 1964. It expressed concern that so little financial support for the Committee had come directly from IUPAC whilst at the same time recognizing the importance of providing advice and services to UNESCO under specific contracts. This concern would be conveyed to the Executive Committee with a request that funds for activities independent of UNESCO should be made available.

International Conference on Laboratory Instruction in Chemistry

Details of this proposed symposium to be held in New York in June 1974 were noted (see pp. 41-42) and the proposal that the symposium should receive IUPAC sponsorship was endorsed.

Survey of Chemistry Teaching at University Level

It was noted, with satisfaction, that the Secretariat had sold 220 copies of the Survey of Chemistry Teaching produced for UNESCO, in the period June 1972-July 1973 and that a further 150 copies had been distributed free of charge, in addition to the 200 copies sent to UNESCO under contract.

Chemical Nomenclature

ASE Booklet. The Committee considered the replies received to the questionnaire sent out by Dr. L. C. CROSS and the Secretary to National Representatives and others interested in chemical nomenclature in chemical education. Also, it received detailed comments from a number of individuals on the booklets by the Association for Science Education in UK on *Nomenclature, Symbols, and Terminology for Use in School Science*.

On balance the Committee felt that the revised ASE booklet, whilst still

not perfect, was worthy of approval as an important contribution towards the introduction of a modern approach to nomenclature at the secondary (school) level. It would wish to encourage the translation of the booklet into other languages, provided suitable safeguards were introduced to assess the accuracy of the translation—perhaps through Members of the Nomenclature Commissions in the countries concerned. The Committee considered that it would be inappropriate, however, for IUPAC to endorse the production of books or guides on nomenclature written by individual authors. One such guide—in Spanish—was submitted for consideration.

The Committee agreed to submit to ASE the detailed comments already received and to convey any further views of the Nomenclature Commissions that might be submitted in the future.

Atomic Weights. The Chairman and Secretary reported their discussions with the Atomic Weights Commission in August 1973 during the XXVII IUPAC Conference as a followup to the recommendation of the Washington meeting (1971) that there should be a simplified version of atomic weight values. It was noted with satisfaction that a Member of the Atomic Weights Commission would prepare four figure numbers as a basis of a simplified atomic weights table and that Prof. N. N. GREENWOOD (Chairman of the Commission) would write an introductory paragraph. This would then be passed to the Members of the Committee for approval and publication in 1974.

International Book Survey

Dr. SYKES reported the results of a questionnaire which he had compiled and distributed on the use of books for chemistry at secondary (school) and tertiary (university) levels. He suggested that there was a clear need for lists of books to be compiled at national level (where this was not already carried out), by national chemical committees or societies and that such lists should be exchanged among the National Representatives. At school level Dr. SYKES would not recommend the establishment of an international exchange scheme for the actual books, but at university level the use of books of foreign origin was much more common and some form of exchange of publications might be valuable. In the majority of instances the use of a chemistry book in a translated edition was as a result of translation from an English or American text.

International Newsletter on Chemical Education

Prof. RAO presented a draft of a newsletter on chemical education which he had compiled from information received from some National Representatives as well as from the Members of the Committee and the Secretariat. The Committee expressed considerable pleasure with this draft and agreed that the publication of such a newsletter, perhaps two or three times per year, would meet a real need for dissemination of information among chemical educators throughout the world.

In view of the support given to the idea of a newsletter at the International Congress on Chemical Education (Recommendation 1.3.3) the Committee expressed the hope that the initial costs of printing and distributing a newsletter might be met by a specific contract with UNESCO for this purpose. The desirability of printing in India was duly noted.

Relations with Other IUPAC Bodies

(i) The Chairman and Secretary reported on their discussions during the XXVII IUPAC Conference with the Teaching Commission of the Clinical Chemistry Section and with the Commission on Analytical Radiochemistry and Nuclear Materials (V.7).

(ii) It was agreed that relations with other IUPAC Commissions interested in specific aspects of teaching chemistry should be fostered and that reports of meetings should be exchanged, possibly through the Secretariat. In particular, the activities of the Commission concerned with teaching of clinical chemistry were noted with great interest, especially the draft of a review monograph on teaching of clinical chemistry to be published jointly in due course by IUPAC and IFCC.

(iii) Also, it was agreed that copies of the report of a conference on the teaching of radiochemistry in schools and colleges, organized jointly by UNESCO and IAEA in Bangkok in 1968, should be sent to the Officers of Commission V.7 and, if possible, to National Representatives and Members of the Committee.

(iv) The Chairman referred to correspondence with the Secretariat and with Prof. G. M. SCHWAB concerning the publication of a textbook on the teaching of colloid and surface chemistry prepared by the IUPAC Commission on the subject. The Committee endorsed the view that such books should be encouraged for commercial publication but not subsidised from IUPAC resources and not designated as officially approved by the Union. They should, however, be listed.

Relations with Advisory Committee on Biochemical Education

The Committee received with interest copies of newsletters and *Biochemical Education*, published by the Advisory Committee on Biochemical Education of IUB. These developments in the teaching of biochemistry were regarded as of considerable help and significance in the overall drive to improve the teaching of chemistry at various levels and it was agreed that closer links should be established between the IUB Advisory Committee and the IUPAC Committee on Teaching of Chemistry. The IUPAC Committee's proposed chemical education newsletter would clearly be able to carry information on biochemical education and likewise the *Biochemical Education* journal would be able to disseminate information on chemical information.

ICSU Committee on Science Teaching

The Secretary reported on recent activities of the ICSU Committee on Science Teaching, particularly on the International Conference on Education of Teachers for Integrated Science held in Maryland, USA, in April 1973. It was agreed that copies of the Report of that Conference should be sent to all National Representatives.

Reference was also made to a symposium to be arranged by ICSU in Spring 1974 on Interpretation, Coordination or Differentiation of the Sciences at University Level, at which it was hoped that the teaching committees of the individual Unions would present their views.

It was noted that the report of the Symposium on Educational Technology sponsored jointly by UNESCO and ICSU (September 1972) would shortly be published in the UNESCO New Trends series, and it was agreed that copies should be made available to Members of the Committee, particularly

in view of the proposal that a symposium on this topic with special reference to chemistry might be held in 1975 in conjunction with the next IUPAC Conference.

Date and Place of Next Meeting

It was agreed that the Committee should meet in Spain in September 1975 and that a symposium should be arranged at the same time. It was also noted that a planning meeting with UNESCO might be convened in May 1975 to advise UNESCO on the longterm planning of activities in chemical education for the biennium 1977-1978.

D. G. CHISMAN

SOLUBILITY DATA PROJECT

The newly established IUPAC Sub-Commission on Solubility Data, in cooperation with CODATA and the Gmelin-Institut of the Max-Planck-Gesellschaft zur Förderung der Wissenschaften, is undertaking a major project on compilation, tabulation, critical evaluation, and publication of solubility data in all physical systems including gases, liquids, and solids.

CODATA will ensure that the usefulness of the scientific material generated by the project is not restricted to users in chemistry and chemical engineering, but also to represent a reliable scientific information of interest to science, medicine, technology, and engineering in general. Gmelin-Institut will undertake the technical editing, publishing, and marketing of the volumes.

The scientific responsibility will be solely that of IUPAC. The Sub-Commission is now recruiting compilers and evaluators, motivated experts who wish to contribute to the success of the project by doing scientific work in their specific field of interest.

For further information please contact:

Prof. A. S. KERTES
Institute of Chemistry
Hebrew University
Jerusalem, Israel

REPORTS OF IUPAC-SPONSORED SYMPOSIA

INTERNATIONAL CONFERENCE ON PROGRESS AND FUTURE OF MACROMOLECULAR SCIENCE

High Tatras, Štrbské Pleso, 15-17 May 1973

Although the correct estimation of the trends of future development of individual scientific fields is extremely difficult, it is still of major importance for countries with limited resources for research. There are several possibilities of solving this problem, but the organization of a conference on the matter appears to be the most suitable one. Such conferences are rarely held in USA. It was the Polymer Institute of the Slovak Academy of Sciences in Bratislava, which filled the gap so far existing in this field by organizing this particular IUPAC-sponsored International Conference.

There are two aspects enabling the Conference to be looked upon as an international scientific event. Firstly, the preparations were arranged by the Commission for Macromolecular Compounds of USSR (Moscow), Centre de Recherches sur les Macromolécules (CNRS Strasbourg), and the Institute of Macromolecular Chemistry (Prague). Secondly, outstanding scientists from the field of macromolecular chemistry from North America and Europe were invited as main lecturers of the Conference. The Conference itself was of a discussion character with only lucid reports on preparation and study of properties of macromolecular systems presented.

A survey of the preparation and development of polymers with inorganic atoms in the main chain (particularly silicon and aluminium) was given by Academician K. A. ANDRIANOFF (USSR). The lecture was read by Prof. V. V. KORSHAK, substituting for Academician ANDRIANOFF who was ill, and dealt with double chains, one inorganic and the other organic. Preparation and study of polyampholytes on the basis of *N*-isopropylcarboxyethylene amine was the concern of Prof. G. SMETS (Belgium) who, in the physicochemical part of his lecture, concentrated on the study of dissociation and complex equilibria of polyampholytes on the basis of the mentioned monomer.

Prof. V. V. KORSHAK (USSR) dealt with polycondensation reactions in polymer preparation. In his broadly conceived lecture, he evaluated both the advantages and the limiting factors of this method of polymer preparation. A survey of the contemporary state of radical polymerization was presented by Prof. F. TÖDÖS (Hungary). In his paper, he reported on the development of production via radical polymerization of mass-produced polymers and outlined possible trends of further development. Preparation of copolymers alternating with metal catalysts of various types was the main concern of Prof. J. FURUKAWA (Japan), who exemplified factors affecting the course of alternating copolymerization, such as polarity, spherical hindrances, and coordination of catalyst.

Dr. J. PRESTON (USA) brought closer the most topical research made in the field of high-strength fibres from wholly aromatic polyesters and showed potential possibilities of their utilization. Macromolecules as agents in organic reactions were dealt with by Prof. C. G. OVERBERGER (USA), who showed possibilities of catalysis by these agents. The problem of possible preparation of artificial enzymes was dealt with by Prof. V. A. KABANOFF (USSR), who concentrated on mathematical modelling of functional activity

of enzymes as the first inevitable degree of artificial enzyme synthesis.

New problems arising in the interpretation of thermodynamic properties of dilute solutions were analysed by Prof. H. BENOIT (France), who focused his attention on the influence of branching on both the thermodynamic and hydrodynamic properties of the solution, as well as on the dependencies of preference sorption parameter on molecular weight. The influence of high pressure on macromolecular solutions was elucidated by Prof. S. CLAESSON (Sweden), who evaluated the contemporary state of experimental techniques of high pressure application in various methods of the study of solution properties of polymers and, with examples from the study of phase equilibria and transitions, he proved the importance of this variable.

Prof. M. KRYSZEWSKI (Poland) dealt with new methods of investigation of electrical properties of polymers, their advantages and limitations, as well as with the possibilities of characterization of the structure of the polymer systems investigated. The relationship between the change of supermolecular structure and chemical transformations of polymers was solved by Dr. B. PHILIPP (GDR) who, with several cases from current practice of cellulose transformations, presented the importance of this parameter in the study of transformation reactions.

Quite a valuable contribution was made by the panel discussions, where, apart from the analysis of problems suggested in the main lectures, prepared communications on topical problems but not included in the main lectures, were read. In the course of the Conference, four panel discussions were held on the following subjects:

New Trends in Macromolecule Synthesis—Discussion leader Prof. A. D. JENKINS (UK)

New Trends in Macromolecule Transformations—Discussion leader Dr. A. CHAPIRO (France)

New Properties and Functions of Macromolecules and Their Systems—Discussion leader Prof. C. G. OVERBERGER (USA)

New Methods of Macromolecular Systems Investigation—Discussion leader Prof. H. J. CANTOW (GFR).

As emphasized in the final evaluation presented by Prof. BENOIT, President of the IUPAC Macromolecular Division, the Conference helped to elucidate the contemporary state, particularly in the field of polymer synthesis as well as that of their physicochemical study. Because of time shortage, less attention was given to polymer physics. The Conference made it possible to foresee the probable further development of macromolecular science.

A. ROMANOV

XI EUROPEAN CONGRESS ON MOLECULAR SPECTROSCOPY

Tallinn, 28 May-1 June 1973

The Congress was organized by the Academy of Sciences of the USSR and Academy of Sciences of the Estonian SSR, and sponsored by IUPAC and the European Physical Society. Delegates came from 22 countries: USSR—384, Poland—34, GFR—29, USA—29, France—28, Czechoslovakia—24, GDR—15, Hungary—14, Italy—11, Netherlands—11, UK—8, Switzerland—

4, Sweden—4, Finland—3, Australia—2, Belgium—2, Bulgaria—2, Spain—2, Denmark—2, Japan—1, Canada—1, Romania—1.

The programme of the Congress included invited review papers and short communications on original research in optical spectroscopy of molecular crystals, impurity molecules and molecular aspects of point defects in ionic crystals, matrix spectroscopy of molecules, intra- and intermolecular energy transfer, Fourier transform techniques and pulse methods in nuclear magnetic resonance (NMR), heteronuclear magnetic resonance of liquids.

The Organizing Committee selected 400 reports, from which 160 were accepted for oral presentation: the abstracts of the rest of the reports were published in a booklet. Some 19 more general reports were presented as plenary lectures and these will be published in the IUPAC journal, *Pure and Applied Chemistry*, during 1974.

Prof. V. L. BROUDE and Prof. E. I. RASHBA (USSR) presented an analysis of the contemporary theoretical and experimental investigations of the exciton spectra of pure and mixed organic molecular crystals. A whole complex of methods available for the determination of the exciton band parameters by the absorption and luminescence spectra was discussed. These methods are essentially based on the describing of intramolecular phonons as stable quasi-particles and on the considering of vibronic states as belonging to the system of the interacting excitons and phonons.

Prof. R. R. ERNST (Switzerland) discussed the equivalence of Fourier spectroscopy and slow passage experiment in NMR. In many important cases, such as the double resonance and the chemically induced dynamical nuclear polarization experiments, these two techniques were shown to be nonequivalent.

Dr. R. FREEMAN and Dr. H. D. W. HILL (USA) discussed various methods of measurement of the spin-lattice relaxation data in liquids with the Fourier transform technique. This technique is particularly useful for carbon-13 relaxation data measurements in complicated organic molecules.

Dr. P. AVAKIAN (USA) gave an interesting review of the influence of magnetic fields on luminescence involving triplet excitons in organic crystals. Even at high temperatures the delayed fluorescence arising from the triplet-triplet annihilation, as well as the hetero-annihilation of free and trapped triplets and the injection of triplet excitons into the crystal with adsorbed dye molecules, can be influenced rather strongly by moderate magnetic fields. Here the features of the processes, not indicated by other methods, are revealed.

Prof. R. M. HOCHSTRASSER (USA) reported on the experimental studies of the triplet exciton bands of molecular crystals. He made a summary of the optical experiments exposing the exciton band structures of the systems of an essentially linear chain exciton character. In his treatment he used the conceptions of energy transfer topology—the effective dimensionality of the exciton, and of cluster states. Also, the use of carbon-13 transitions in the study of the details of the exciton band, the use of heavy doping as a band structure indicator, and the application of two-photon spectroscopy to the study of triplet excitons were discussed. His report included a lot of new material and new ideas.

Prof. M. TRLIFAJ (Czechoslovakia) made a survey of the results of the theoretical study of the exciton-exciton interactions in molecular organic crystals. The bound states of two excitons (biexcitons), caused by cubic and quartic inharmonic interaction between electron excitations in the crystal, were considered. Their coherent and incoherent motion models were dis-

cussed. Also, the annihilation of two excitons as a bimolecular decay process, resulting in an uncharged or charged electron excitation, was considered.

Prof. K. K. REBANE and Dr. L. A. REBANE (USSR) summarized the present status and results of the investigations of small molecular ions as impurity centres in crystals. They reviewed the physical results of the structure of centres, the electronic, vibrational and vibrational-rotational states, and the relaxation processes in impurity centres. The investigation of the impurity-crystal interaction and the local dynamics of the crystal lattice were also discussed. The comprehensive data of the spectra of infrared absorption, vibronic absorption, luminescence and Raman scattering, and the spectra of vibronic, rovibronic and infrared hot luminescence, were used.

Dr. N. KRISTOFFEL and Dr. G. LIIDJA (USSR) spoke of various molecular aspects in the theory of usual impurity centres (substituted ions) in alkali halides and of the intrinsic electron excitations in these crystals. They pointed out that at the present time a number of problems in the theory of impurity centres (the theory of the shape of vibronic spectra, resonant Raman scattering, radiationless transitions, *etc.*) seemed to be elaborated far more thoroughly than in the theory of polyatomic molecules, and the introduction of the corresponding results into the theory of molecular objects was topical.

Quite a few reports at the Congress were dedicated to Shpol'skii systems. Prof. E. V. SHPOL'SKII and Dr. T. N. BOLOTNIKOVA (USSR) summarized and systematized the theoretical and experimental data of the investigation of luminescence and absorption spectra of different organic substances in frozen polycrystal solutions. In the analysis of the quasilinear spectra of these systems the conception of quasilinear spectrum as the optical analogue of the Mössbauer effect has been stimulating. It was underlined that the peculiarities of quasilinear spectra (the well resolved vibrational structure and the sensitivity to internal and external perturbations) make it possible to use them in solving different problems of molecular and crystal spectroscopy.

A review lecture about optical properties in connection with molecular interactions was given by Prof. B. VODAR (France). Prof. B. S. NEPORENT (USSR) reviewed the results of spectroscopic investigations of intramolecular vibrational and electronic relaxations in organic complex molecules. A model of a polyatomic molecule, permitting one to follow the basic features of the relaxation process, was discussed.

Prof. M. V. VOLKENSTEIN (USSR) gave a special lecture about the Faraday spectroscopy of proteins as of aperiodic molecular crystals. Prof. K. WÜTHRICH (Switzerland) gave a short survey of recent developments in the NMR spectroscopy of peptides and proteins. The report was illustrated by some new experimental data of carbon-13 magnetic resonance in cyclic peptides and haemoprotein.

The authors of many reports underlined the biological aspects of their investigations.

A new kind of light scattering—the vibro-electronic Raman effect—has been observed in the impurity crystal by C. KANE-MAGUIRE and Prof. J. A. KONINGSTEIN (Canada). Dr. P. M. RENTZEPIS (USA) spoke about an excellent method of application of picosecond pulses (generated by mode-locked lasers) for the study of ultrafast relaxation processes in organic and biological molecules. The power of the method was demonstrated on a number of direct observations of radiative and radiationless transitions in liquids. The methods of simultaneous time-frequency resolved emission and absorption spectra allowed one to measure with a time resolution limited by the time length of the picosecond pulse.

In a number of investigations reported at the Congress phosphorescence-microwave double resonance (PMDR) methods were applied. Prof. C. B. HARRIS (USA) reported the PMDR in exciton states of molecular crystals and coherent states of triplet spin ensemble. Prof. D. M. GRANT (USA) made an excellent review of the chemical and physical aspects of carbon-13 NMR spectroscopy. Carbon-13 NMR spectroscopy was recommended as an effective method of studying molecular structure and molecular dynamics in liquids. Dr. M. WITANOWSKI (Poland) summarized the results of nitrogen magnetic resonance spectroscopy studies in organic liquids. Dr. V. S. PETROSYAN and Prof. O. A. REUTOV (USSR) reported on some aspects of the NMR of heavy atoms, such as tin, platinum, and mercury, in organic and inorganic compounds.

T. SALUVERE
O. SILD

XV INTERNATIONAL CONFERENCE ON COORDINATION CHEMISTRY

Moscow, 25-30 June 1973

The Conference was organized by the Academy of Sciences of USSR and the Lomonosov Moscow University and sponsored by IUPAC and the State Committee of Council of Ministers of the USSR on Science and Engineering.

The delegates came from 29 countries: USSR—838, Czechoslovakia—54, Poland—39, USA—38, Italy—25, GFR—20, France—20, Hungary—18, Sweden—16, GDR—14, Japan—13, Switzerland—13, Romania—11, Bulgaria—8, Denmark—6, UK—6, Canada—5, Yugoslavia—4, Australia—3, Finland—3, India—3, Brazil—2, Greece—2, Austria—1, Belgium—1, Iran—1, Ireland—1, Netherlands—1, Spain—1 (the total number was 1167).

The scientific programme included reports on spectroscopy of coordination compounds; structure and bonding in coordination compounds; synthesis of new types of coordination compound; thermodynamics, kinetics, and mechanisms of complex formation; catalysis with coordination compounds; and complex formation in nonaqueous solutions and gaseous phase.

At the Conference there were presented: plenary lectures—13 (under course of publication in *Pure and Applied Chemistry*), section lectures—27, section reports—386. Some 597 abstracts were published.

At the L. A. CHUGAEV Centenary Memorial, N. M. ZHAVORONKOV (USSR) made a report in honour of the great scientist. He spoke on the main aspects of CHUGAEV's versatile scientific activity. He characterized CHUGAEV as an outstanding scientist, who made a great contribution to the development of coordinating chemistry and whose works dealing with complex compounds were still of great significance today. J. C. BAILAR, JR. (USA), in an interesting lecture about CHUGAEV, pointed out that coordination chemistry was only one of the fields in which he had worked. He noted that CHUGAEV had made important contributions in organic chemistry, in physical chemistry, and also published some significant papers on analytical topics. S. A. SCHUKAREV (USSR) spoke about personal recollections, referring to the period of CHUGAEV's activity as a head of the Mendeleev chair

of chemistry at Leningrad University. He characterized CHUGAEV as a brilliant lecturer and a talented student educator, and as a progressive scientist bringing up perspective problems.

Many reports at the Conference were devoted to theory and experimental data on structure and bonding in coordination compounds. The modern state of electronic structure calculations for coordination compounds of nontransition, transition, and heavy elements was reviewed in the plenary lecture of M. E. DYATKINA,* N. M. KLIMENKO, and E. L. ROZENBERG (USSR). Application of calculations for quantum chemical studies of bonding problems and for interpretations of molecular properties (e.g., charge distributions, dipole moments, ionization potentials) was also discussed. The consideration of modern quantum chemistry calculations was illustrated with examples taken from the literature and with the authors' own results.

J. GAŽO (Czechoslovakia) analysed a special case of space isomerism, so-called 'distortion isomerism', showing different physical and chemical properties of the respective isomers (colour, spectral properties, magnetic behaviour, thermal stability, and chemical reactivity.) L. BAKER (USA) reported on new discoveries in the field of heteropolycompounds.

V. I. SPITSYN (USSR) gave a review of ionizing radiation action on coordination compounds. The stability of inorganic salts to radioactivity is determined by many factors, including the complex composition and the nature of the metal-ligand bonds. The author with his assistants had found that the radiation stability of platinum complexes depends on the oxidation state of the central ion and redox M—L interaction. Iodine containing lead (IV) complexes have the lowest radiation stability.

B. JEŹOWSKA-TRZEBIATOWSKA (Poland) spoke about complex compounds as models of biologically active compounds. Her report included some aspects of cobalt, iron, and copper complex activity because they, among all other transition metals, play the main role in the metabolic processes. The mechanism of reversible uptake of molecular oxygen and nitrogen fixation in systems similar to those in nature was discussed. Investigations of models of oxygen-containing systems made it possible to find new synthetic systems which reversibly took up molecular oxygen in aqueous and nonaqueous solutions. These were cobalt(II) complexes, containing aminoacid or dipeptide molecules and imidazole, as ligands.

The ligand mutual influence in coordination compounds presents one of the most important problems in coordination chemistry. K. B. YATSIMIRSKII (USSR) discussed kinetic and thermodynamic aspects of this vital problem, having shown the ways of ligand *trans*- and *cis*-influence in coordination compounds of transition metals.

L. CATTALINI (Italy) gave a thorough analysis of square planar four-coordinated complexes of Pb(II), Pd(III), Au(III), Rh(II), etc. He gave an account of the main factors determining the reactivity of such complexes. D. STRANK's (Australia) works added new data to the knowledge of ion hydrotation and sequence of aquatation processes. The author had reached the conclusion that there are two shells of water molecules around a charged complex in solution (ML_6^{3+}). Their molar volume and compression is less than the bulk water in the solution.

K. SAITO (Japan) had come to the opinion that, in order to explain some reaction mechanisms, it is necessary to acknowledge β -diketonates ability as

*Deceased

a monodentate ligand. Isotopic exchange investigation makes it possible to get important data about the reaction mechanism, *i.e.*, ligand behaviour in substitution reactions. The use of β -diketonates, enriched by carbon-14, helped scientists to study exchange reactions of different diketonates of In(III), Ga(III), and Al(III). G. WILKE (GFR) in his report analysed the optically active complexes and catalytic indication of the asymmetric ion.

The growing level of studies of complexes, which was widely shown at the Conference, makes it possible to expect further new achievements in this field of inorganic chemistry.

YU. A. BUSLAEV

INTERNATIONAL SYMPOSIUM ON MICROCHEMICAL TECHNIQUES—1973

University Park, Pennsylvania, 19-24 August 1973

This Symposium was held on the campus of Pennsylvania State University and was conducted by that University through its College of Science. It was organized by the American Microchemical Society with the sponsorship of the Commission on Microchemical Techniques and Trace Analysis of the Division of Analytical Chemistry of IUPAC.

Scientists from 17 countries attended, coming from as far away as Australia and Japan. Rather large delegations were present from Austria, Canada, Germany, Switzerland, UK, and, of course, USA. The other countries represented were Denmark, France, Greece, Italy, Netherlands, Spain, and Sweden. The total attendance of registered scientists was 260, 64 of whom were from countries other than USA. The actual attendance, including guests (wives and children), totalled about 340.

Like the previous three Symposia held at Pennsylvania State University (1961, 1965, and 1968), the speakers were of international reputation and authorities in their respective fields, which included a number of branches of science involving small-scale manipulation.

Ninety-seven papers were presented, covering the subjects of organic functional group analysis, thermal methods of analysis, forensic analysis (narcotics and drugs of abuse), automated elemental analyzers, trace analysis, microelectrodes, new techniques in microchemistry, computers in the laboratory, standards and standardization for microchemistry and microanalysis, the art of presenting a paper, new methods for organic elemental analysis, clinical and biochemical techniques, environmental analysis, ion selective electrodes, and computerization of a commercial elemental analyzer. Thirteen commercial exhibitors displayed many of the pieces of apparatus discussed in the technical sessions. This often served the purpose of demonstrating the methods discussed in the papers presented in the technical sessions.

The use of various chromatographic methods was stressed and the papers indicated an ever increasing use of automation involving the use of computerization. In spite of this trend, classical methods do not seem to be losing ground. The session entitled 'The Art of Presenting a Paper' was well attended

and was most informative. It would be most difficult to 'label' any one session or paper as the 'highlight'. If no papers had been presented and the group had gotten together to hold informal discussions, the calibre of those present would have ensured the success of the Symposium. The success of the past Symposium warrants the holding of others in the future with the sponsorship of IUPAC.

A. STEYERMARK

PRAGUE MEETINGS ON MACROMOLECULES—1973

The XII Microsymposium on Macromolecules, entitled 'Organized Structures in Polymer Solutions and Gels', was held during 20-23 August 1973 at the Institute of Macromolecular Chemistry of the Czechoslovak Academy of Sciences in Prague. The number of active participants was 136, representing 16 countries. The meeting was opened on behalf of IUPAC by Prof. H. BENOIT, President of the IUPAC Macromolecular Division. Nine main lectures and 52 short communications were delivered at the Microsymposium. The main lectures will be published in the official IUPAC journal *Pure and Applied Chemistry*. Some of the short communications will appear in *Journal of Polymer Science, Part C (Polymer Symposia)*. The Opening Lecture was presented by H. BENOIT (France) and dealt with the elucidation of the effect of incompatibility on the structure of block copolymers in solution. He summarized what was known so far about the properties of copolymers, particularly in dilute solutions, and what problems still remained to be investigated. The lecture given by B. GALLOT (France) dealt with periodic structures exhibited by block copolymers in both the liquid and the solid states. Investigations by differential scanning calorimetry, low angle X-ray diffraction, and electron microscopy, have established the occurrence of five types of periodic structure differing in their geometry.

The lecture by F. D. SAEVA (USA) was devoted to the results of the study of liquid crystalline mesophases of the cholesteric type. Liquid crystal induced circular dichroism (together with other methods) was used to probe the internal molecular organization of cholesteric mesophases. The thermodynamics and dynamics of solutions of poly- γ -benzyl-L-glutamate were the topics of the lecture by W. G. MILLER (USA). The experimental results (obtained by thermodynamic, hydrodynamic, and spectrometric methods) were compared with predictions based on the theory of solutions of rigid polymer chains. The differences found were correlated with the deviations from rigid rod behaviour and with the importance of flexible side chains.

The behaviour of liquid crystals of biological importance (*i.e.*, the melting process associated with the lipid chains at temperatures below the final melting point of phospholipids and glycolipids and the lyotropic mesomorphism in the presence of water) was discussed by D. CHAPMAN (UK). The importance of these phenomena for the structure and function of cell membranes was emphasized. The lecture by KANG-JEN LIU (USA) reviewed the author's results obtained by the NMR technique in the investigation of the solvent effect on the conformation of macromolecules and of the interaction of solvent molecules with different functional groups in the polymer chains. New NMR and viscosity data presented by Dr. LIU were an important contribution to the elucidation of the association of polymethylmethacrylate molecules.

Nucleation and crystal growth in polymer solutions was the subject of the lecture by H. G. ZACHMANN (GFR). A new theory of these processes was presented which makes it possible to explain the influence of various factors (e.g., supercooling, concentration, molecular weight, *etc.*) on the kinetics of crystallization and on crystal properties. The usefulness of the method of pulse-induced critical light scattering for the investigation of critical states in polymer solutions was demonstrated by M. GORDON (UK). The method is a very powerful tool in providing new information on phase equilibria and kinetics of phase changes in polymer solutions.

In the closing lecture S. YA. FRENKEL (USSR) presented essential features of his thermokinetic approach to the formation of organized structures in polymer solutions. Based on this approach the author made an attempt to 'bring to a common denominator' the phenomena discussed in the Microsymposium.

The XIII Microsymposium on Macromolecules, entitled 'Transformation of Functional Groups on Polymers', was held from 27 to 30 August 1973, at the same place as the preceding Microsymposium. Prof. C. G. OVERBERGER represented IUPAC at this meeting. Of nine invited main lectures, eight were delivered (Prof. V. A. SERGEEV could not participate). The total number of communications (67) and of active participants (175 from 17 countries) was somewhat 'supercritical', but did not lead to any major disturbances in the programme. Both main lectures and short communications will be published similarly to the preceding Microsymposium.

The Opening Lecture by C. G. OVERBERGER (USA) was devoted to the main differences between low-molecular-weight and polymeric transformations. Cooperative effects were discussed in connexion with the specificity of polymeranalogous reactions. The effect of both electrovalency interaction and weak interaction on the specificity of sorption in weak acid cation exchangers was demonstrated by G. V. SAMSONOV (USSR). The systems under investigation included new types of crosslinked carboxylic polyelectrolyte, antibiotics, enzymes, and protein hormones.

The lecture by O. WICHTERLE (Czechoslovakia) dealt with polymeranalogous transformations limited to a thin surface layer of the polymer. Thin layers exhibiting a specific chemical or biological activity on an inert substrate whose function was purely mechanical were of primary interest. G. MANECKE (GFR) discussed polymers with reversibly oxidizable and reducible redox groups on a crosslinked matrix. Synthesis, electrochemical properties, and applications of redox resins were described.

The topic of the lecture by F. TÜDÖS and T. KELEN (Hungary) was the polymeranalogous reactivity of polyenes formed during the thermal degradation of polyvinyl chloride. The low-molecular-weight reactants included hydrogen chloride and dienophilic reagents. R. C. SCHULZ (GFR) described several examples of complexes between polymers and low-molecular-weight compounds: lanthanide complexes with polyacetals, iodine complexes with polyvinyl alcohol and polyethylene oxide, metal complexes with polysaccharides, amylose complexes with azo compounds, and donor-acceptor complexes. The lecture by R. J. P. WILLIAMS (UK) dealt with the nature of the binding sites of metals in proteins and enzymes. The aim of the lecture was to conceive of methods for making synthetic polymers with high catalytic activity.

The closing lecture by H. MORAWETZ (USA) considered the influence of polymeric chain conformations on the reactivity of functional groups. Re-

actions involving two functional groups on the same or on different polymeric chains were discussed.

The organization of both Microsymposia was similar to previous years: the main lectures, short communications, and discussion sessions were each allotted approximately one third of the programme.

M. BOHDANECKÝ
B. SEDLÁČEK
J. ŠTAMBERG

**III INTERNATIONAL CONFERENCE ON
CHEMICAL THERMODYNAMICS**
jointly with
**SYMPOSIUM ON PHYSICOCHEMICAL
TECHNIQUES AT HIGH TEMPERATURES**
Baden near Vienna, 3-7 September 1973

The Conference was organized by the Austrian Chemico-Physical Society and sponsored by IUPAC. The scientific programme contained six plenary lectures and the original contributions were grouped into eleven sections.

The plenary lectures were as follows:

Polar and Ionic Fluids at High Temperatures and Pressures E. U. FRANCK (GFR)
Phase Equilibria in Condensed Systems O. KUBASCHEWSKI (UK)
Equilibria between Fluid Phases in Mixtures of Nonelectrolytes J. S. ROWLINSON (UK)
Liquid Crystals H. SACKMANN (GDR)
Biochemical Thermochemistry I. WADSÖ (Sweden)
Calorimetry of Phase and Ordering Transitions E. F. WESTRUM, JR. (USA)

The eleven sections were organized by programme chairmen as follows:

Calorimetric Techniques and Apparatus M. LAFFITTE (France)
Thermochemical Quantities, including Enthalpies of Combustion of Reacting Systems J. D. COX (UK)
Thermodynamic Properties of Pure Fluids J. W. PERRAM (Australia)
Thermodynamics of Fluid Mixtures (Nonassociating Components) A. G. WILLIAMSON (New Zealand) and K. N. MARSH (Australia)
Liquid Mixtures with Associating Components (Nonelectrolytes) H. V. KEHIAIAN (France)
Solutions of Electrolytes (including Polycondensations) G. CARPÉNI (France) and P. HUYSKENS (Belgium)
Mixtures of Metallic and Ionic Melts S. STERNBERG (Romania)
Thermodynamics of Interfaces G. H. FINDENEGG (Austria)
Thermodynamic Properties in Solid Single and Multicomponent Systems K. L. KOMAREK and A. NECKEL (Austria)
Thermodynamics of Systems of Biochemical Interest H. RÜTERJANS (GFR)
Compilation and Tabulation of Thermodynamic Data S. ANGUS (UK)

The Symposium on Physicochemical Techniques at High Temperatures was divided into the following six sections:

Temperature Production and Measurement
Vapour Pressures and Gas-condensed Phase Equilibria
Structural Studies by X-ray Diffraction
Calorimetry
Electromotive Force Measurements
Kinetic Studies

Short versions of all papers are in process of being published in *Canadian Metallurgical Quarterly*.

The sections of the Conference and the Symposium were run in three parallel sessions. A total of 264 papers was presented. The six plenary lectures from the Conference are to be printed in the IUPAC journal, *Pure and Applied Chemistry*, and published as a special bound reprint from Butterworths (London). Manuscripts of all other papers were printed by the photographic reproduction method and issued as preprints in eight bound volumes at the beginning of the Conference.

The social programme included receptions by the Landeshauptmann of Lower Austria and by the Mayor of Baden. Private discussions between the participants were stimulated by making two afternoons free. Also, it is hoped that the surroundings of Baden, which is a lovely watering place on the slope of the Viennese Woods, already known to the Romans, contributed to this aim.

The Conference was attended by 370 active participants from the following 31 countries: Austria, Australia, Belgium, Bulgaria, Canada, Czechoslovakia, Ecuador, France, German Democratic Republic, German Federal Republic, Greece, Hungary, India, Israel, Italy, Japan, Mexico, Netherlands, Norway, Poland, Portugal, Romania, Spain, South Africa, Sweden, Switzerland, Turkey, UK, USA, USSR, and Yugoslavia.

G. FINDENEGB
F. KOHLER

INTERNATIONAL SYMPOSIUM ON MACROMOLECULES

Aberdeen, 10-14 September 1973

In the past, this series of symposia has concentrated almost exclusively on the more academic aspects of macromolecular research and on the more chemical lines of advance. This year's Programme Committee, chaired by Prof. C. E. H. BAWN, determined that the meeting should endeavour to promote papers and discussion in more applied areas such as the manufacture and processing of polymeric materials. While this innovation—possibly for real or imagined reasons—was not as successful as had been hoped, it did constitute a substantial deviation from the accepted pattern and should lead to a further broadening of the basis of the symposia.

The official opening, performed by the Rt. Hon. GORDON CAMPBELL, Secretary of State for Scotland, was preceded by a degree ceremony at which the University conferred honorary Doctorates in Science on Prof. H. BENOIT (Strasbourg) and Prof. G. SMETS (Louvain), respectively, President and Secretary of the Macromolecular Division of IUPAC. There were over 900 registered delegates and accompanying members, coming from 30 different countries, with large contingents from Eastern Europe and Japan.

The Symposium was divided into seven sections which operated simultaneously, each session dealing with a coherent group of papers. A feature of the proceedings was the large number (45) of longer discourses given by eminent workers in various fields. These longer papers were interspersed throughout the programme and, although very well attended, did not detract too much from the shorter communications made simultaneously. The invited lectures are to be published in the IUPAC journal, *Pure and Applied Chemistry*.

The synthetic section included papers on high temperature adhesives (C. S. MARVEL, Arizona), cyclopolymerization (T. SAEGUSA, Kyoto), asymmetric polymers (C. G. OVERBERGER, Michigan), and reactions in solid polymer systems (G. SMETS, Louvain); while C. H. BAMFORD (Liverpool) and G. M. BURNETT (Aberdeen) concentrated on aspects of crosslinking. On polymer properties, special emphasis was given to polymer compatibility (R. KONINGSVELD, Geleen), the inter-relation of polymer structure and rheological properties (G. V. VINOGRADOV, Moscow), the properties and structure of block copolymers (H. BENOIT, Strasbourg), behaviour of polymers in multiaxial stress states (S. S. STERNSTEIN, Troy), relaxation in relation to environment (A. M. NORTH, Strathclyde), fracture mechanics (J. G. WILLIAMS, London), and elasticity in crosslinked polymers (G. REHAGE, Clausthal). Principal contributors on crystallinity and morphology included E. W. FISCHER (Mainz), A. KELLER (Bristol), and E. H. ANDREWS (London).

More industrial and applied contributions came from J. P. HOGAN (Oklahoma) who discussed the Phillips polyethylene process in some detail, and E. W. DUCK (Southampton) who was concerned with a chemical and economic analysis of diene polymerization in solution. G. ALLIGER (Akron) gave a detailed discussion of liquid systems that lead to rubber products, including the manufacture of tyres. Among those contributing to the section on diffusion studies were G. ALLEN (Manchester) who spoke on the application of neutron diffraction to the evaluation of self diffusion in rubber and polymer melts; and P. MEARES (Aberdeen) who proposed a possible molecular interpretation of material transport phenomena in polymers. The last was complemented by a discussion of the influence of morphology on transport in crystalline polymers by A. PETERLIN (Research Triangle Institute). While little time was available for formal discussions there is no doubt that much of the material presented triggered off lively informal exchanges.

Two reports of IUPAC Working Parties were presented in conjunction with the symposium. One was concerned with the dynamic, mechanical, and impact properties of polyvinyl chloride and the other with the effect of molecular orientation on the mechanical properties of polystyrene. Both were the result of large-scale collaborative studies undertaken by laboratories throughout the world.

Another break with tradition was that there was no introductory talk by Prof. H. MARK (ex Brooklyn). Instead he gave a lecture at the end of the proceedings on Polymers in China. Prof. MARK was a member of the US team which recently visited China and was able to discuss at first hand the position with regard both to research on and production of polymeric materials in China.

G. M. BURNETT

INTERNATIONAL CONGRESS ON IMPROVEMENT OF CHEMICAL EDUCATION

Wrocław, 17-22 September 1973

The Congress was organized by the UNESCO Division of Pre-University Science and Technology Education, although the arrangements were put in hand in 1972 when the Division was entitled Division of Science Teaching and embraced both university and preuniversity science education. From 1 January 1973 the new Division had been part of the Education Sector of UNESCO whilst university science education remains under the control of the Science Sector in UNESCO.

A Steering Committee, comprising representatives of the Polish authorities, UNESCO staff, and the IUPAC Committee on Chemistry Teaching, met in Paris in June 1972 when the general structure of the Congress was determined. Since that date the day-to-day arrangements had been in the hands of UNESCO.

The Congress represented one of a series of major review conferences in the UNESCO programme whose aims are to study trends in the teaching of the sciences over a four- or five-year period by means of commissioned trend papers. These papers, as amended at the conference and supplemented by discussions and recommendations for future action, will form the substance for a publication in the UNESCO New Trends series.

About 130 participants attended the Congress, including the authors of the 13 trend papers and Polish chemists, and three UNESCO staff members. Of these, 44 were from Western Europe, 43 from Eastern Europe (23 from Poland), 11 from N. America, 5 from Asia, 6 from Latin America (5 from Argentina), 4 from Caribbean (all from Cuba), 3 from Australasia, 6 from Arab Middle East, and 1 from Africa.

Local arrangements were in the hands of a Local Committee under the Chairmanship of Prof. B. JEŻOWSKA-TRZEBIATOWSKA. Accommodation was dealt with by ORBIS, the Polish travel agency, through whom all financial transactions were conducted. In addition to the professional programme (see below), the Local Committee organized a number of social events, including an orchestral concert, a cocktail party given by the Minister of Chemical Industry and the President of the City of Wrocław, and a Conference Banquet.

The Congress included three plenary sessions on

‘Where is chemistry going’ by Academician N. SEMENOV (USSR)

‘Where is education going’ by Prof. A. KADDOURA (Arab Republic of Syria)

‘Future problems of society of concern to scientists’ by Dr. P. HARPER (UK)

in addition to opening and closing sessions.

However, the main work of the Congress was undertaken in the thirteen concurrent working groups, each related to a trend paper prepared by an author who was specially invited to the meeting. These sessions were concerned with the effect on the design of chemistry courses and programmes of:

- the changing needs and views of society (C. TERLON, France)
- the evolving demands of industry and other professions (E. S. STERN, UK)
- the evolution in the nature and structure of chemistry (B. JEŻOWSKA-TRZEBIATOWSKA, Poland)

- the changing characteristics of students (A. GUERRERO, Argentina)
- updated and more precise learning objectives in chemistry (M. J. FRAZER, UK)
- better understanding of the psychological processes of learning chemistry (U. HOFACKER, Federal Republic of Germany)
- variations in the methods of teaching chemists (S. ACHMAD, Indonesia)
- the enhanced potentialities of new educational technology (C. N. R. RAO, India)

There were also working groups on:

- new approaches to the design and evaluation of chemistry courses (D. COHEN, Australia)
- improved techniques for assessing student achievement (T. ASHFORD, USA)
- trends in the training and retraining of chemistry teachers (A. V. BOGATSKI, Ukrainian SSR)
- varying approaches to promoting improvements in chemical education (G. ILLUMINATI, Italy)
- trends in international cooperation in the improvement of chemical education (R. W. PARRY, USA)

More than fifty recommendations were drafted by the various working groups (see pp. 33-37). These were subsequently arranged into three main sections addressed to international agencies, national organizations, and individual institutions. The proceedings of the Congress will be edited by Dr. P. FARAGO (UK) and published by UNESCO in 1974.

The Congress was undoubtedly successful in the sense that any conference of professionals has enormous value in bringing people together to discuss mutual problems and as an opportunity of exchanging information. The publication of the thirteen commissioned papers, amended in the light of discussions in Wrocław, will also be of great value. The number of participants was fewer than anticipated and their geographical distribution was uneven—only one from Africa, for instance.

It was most unfortunate that the time available to organize the arrangements was short and this fact was aggravated by the delay in printing and distributing the publicity leaflets, particularly the second one giving the registration details and application forms which did not appear until early August 1973—an inopportune time for the majority of academics.

The organizational problems were further complicated by the decision to ask for all replies to the second circular to be sent to UNESCO rather than to Poland and by the insistence of UNESCO in exercising some selection of participants in order to maintain a political or geographical balance. In the event, the Congress was much undersubscribed and the quality of participants was not as high, on average, as might have been expected. In retrospect these aspects might have been better in the hands of the Polish Local Committee or IUPAC.

The presentations of two of the plenary speakers were not as high level as anticipated—the exception was Prof. A. KADDOURA, whose delivery and content were first class. The problem of presentation by Academician SEMENOV was further complicated by a failure of the technical aspects of the simultaneous translation services. It is hoped, however, that the plenary lectures will read well when published.

D. G. CHISMAN

DRAFT RECOMMENDATIONS FROM INTERNATIONAL CONGRESS ON IMPROVEMENT OF CHEMICAL EDUCATION

I. INTERNATIONAL AGENCIES

I.1 Conferences/Meetings

- 1.1.1 Review conferences should be convened internationally every four or five years to assess trends in chemical education and to promote interchange of ideas among national chemical groups. A report to examine progress made in implementing recommendations of the 1973 Congress should be prepared two years after the publication of the proceedings.
- 1.1.2 Regional meetings should be arranged on specific aspects of chemical education. One such meeting should be to assist and give instruction to teachers in formulating aims and objectives of chemical education and translating such aims into meaningful classroom/laboratory action. (The establishment of international committees to formulate precise objectives is *not* recommended.) (See also 2.1).

I.2 Advisory Services

- 1.2.1 Lists of international experts should be compiled so that panels can be set up to respond to requests for assistance in the following areas:
 - 1.2.1.1 *Examinations*—to review and criticize examination procedures, to promote improvement in instruments of assessment, and to facilitate dissemination of currently available instruments. (Note. No attempt to exercise a rigid control of education is envisaged and those elected to serve on the panel should have some knowledge of country or region if invited to comment on its examination system.)
 - 1.2.1.2 *Development and Evaluation of Educational Structures at University Level*—to provide advice on organizational matters, academic terms, and administrative practices of educational institutions. (Note. Not to impose procedures or dictate solutions.)
 - 1.2.1.3 *Correlation of Academic Standards*—To advise on correlation of academic qualifications, for instance the work of the International Baccalaureat and the plans of the Federation of European Chemical Societies.
 - 1.2.1.4 *Continuing Education for Chemists and Chemistry Teachers*—to provide advice and assistance and to disseminate information on experience throughout the world.
 - 1.2.1.5 *Educational Techniques, Methodology, and Equipment*

I.3 Information

- 1.3.1 The international network linking all groups active in the improvement of chemical education should be strengthened in order to facilitate a better exchange of ideas and information through publications and meetings.
- 1.3.2 The collection and dissemination of innovative material on chemical education should be strengthened through the expansion of UNESCO's existing Science Teaching Information Centre.

- 1.3.3 Information on new methods of teaching chemistry should be submitted to IUPAC through national chemical education groups or UNESCO field staff or the IUPAC National Representatives for dissemination through the proposed IUPAC Chemical Education Newsletter.

1.4 Surveys and Investigations

- 1.4.1 Statistical surveys should be commissioned to provide comparative information on an international basis of the output of graduate chemists (after three, four, and six years of university study), the availability of industrial posts for chemists, and the utilization of chemists at all levels.
- 1.4.2 Research investigations into the effect of defining of objectives on the efficiency of learning should be commissioned.
- 1.4.3 Investigations should be commissioned on:
- 1.4.3.1 The applicability of existing theories of educational psychology to chemical education at different levels.
- 1.4.3.2 The conceptual structure underlying chemical knowledge and the relations of chemical concepts to each other.
- 1.4.4 A study should be made of the relationship between brain function and nutritional factors.
- 1.4.5 A study should be initiated to investigate the instructional practices of different curriculum projects to ascertain what psychological generalizations may apply.
- 1.4.6 Data and general information about different aspects of student characteristics should be collected internationally.
- 1.4.7 Multinational experimental studies on the psychological aspects of teaching chemistry should be encouraged.
- 1.4.8 A global study should be undertaken to determine the needs of chemistry teachers, over a period of at least five years, and to evaluate the national possibilities of responding to these needs bearing in mind the economic situations and the availability of international cooperation.
- 1.4.9 A survey on chemical education in developing countries should be commissioned.
- 1.4.10 A survey on chemical education at tertiary level in Europe should be undertaken.

1.5 Publications

- 1.5.1 A study should be published on the effect of chemicals on behaviour *e.g.*, pheromones, mosaics, circadian rhythms, brain chemistry.
- 1.5.2 Articles on chemical education should contrive to be selected, translated, and published as in the early editions of *New Trends* and a bibliography of pedagogical studies in chemistry should be compiled.
- 1.5.3 Reports on experiments in the use of educational technology in the teaching of chemistry should be published and periodic surveys and symposia arranged. The first such symposia should be arranged within the next two years. (See also 2.1)
- 1.5.4 The procedures used in developing chemistry curricula in different projects should be documented fully and published for international reference.
- 1.5.5 An international journal of chemical education should be launched.

- 1.5.6 Articles on teacher training and retraining of chemistry teachers at all levels should be commissioned by UNESCO and published.

1.6 Innovation

- 1.6.1 Competitive grants should be made available internationally and nationally to finance experiments in the design of 'core' courses and 'option' courses that better reflect the changing nature of the structure of chemistry.
- 1.6.2 Regional centres, such as RECSAM, should be established to experiment with and develop new methods of teaching chemistry and to disseminate the results regionally and internationally.
- 1.6.3 An international centre for educational technology should be established for the dissemination of information, for training teachers, and for production of material.
- 1.6.4 Special attention should be given to the use of educational technology in developing countries.

1.7 General

- 1.7.1 UNESCO should attempt to minimize the problems of copyright on 'software', such as films and slides.
- 1.7.2 Exchange of students and teachers of chemistry among nations should be fostered by whatever international or national means available.
- 1.7.3 Combined contributions from experts in the various branches of science should be encouraged in view of the similarities in the mechanisms of change and more opportunities for studying change should be provided. (See also 1.5.4).

2. NATIONAL ORGANIZATIONS

National chemical education groups, committees, or professional bodies, should be established in countries where they do not already exist, to undertake the promotion of international cooperation in chemical education and national activities in the following ways:

2.1 Meetings

- 2.1.1 To organize workshops and courses for chemistry teachers.
- 2.1.2 To organize, in collaboration with other national groups, regional conferences on specific aspects of chemical education. (See 1.1.2).

2.2 Information

- 2.2.1 To prepare lists of chemical educators in each country for mailing purposes and for submission to international agencies for computer storage.
- 2.2.2 To prepare lists in appropriate languages of books and articles on improvement of chemical education within the different countries.

2.3 Innovation

- 2.3.1 To arrange for the assessment of new techniques in chemical education, such as self-paced learning and open-ended laboratory instruction.
- 2.3.2 To provide a link between chemists and educators to foster greater

cooperation and understanding between these two groups. For instance, educators should periodically be involved in the work of university chemistry departments, and scientists as well as administrators should be involved in the development of curriculum projects.

- 2.3.3 To provide greater opportunities for studying mechanisms of change in chemical education, through articles, conferences, and comparative studies with other countries. (See also 1.7.3)

2.4 Studies and Publications

- 2.4.1 To study the different methods of training chemistry teachers for different levels of education through universities and colleges of education and to review experience obtained from retraining chemistry teachers.
- 2.4.2 To encourage the publication of monographs on new techniques and methods of teaching chemistry.
- 2.4.3 To monitor experiments in the use of satellites for chemical education both for students and for the general public.

2.5 Science Teaching Centres

- 2.5.1 To support and strengthen the international activities of national centres for chemical education or science education.
- 2.5.2 To stimulate the establishment of a national centre for educational technology which might act as a clearing house for experiments in the use of educational technology both for conventional courses and for continuing education.

2.6 General

- 2.6.1 To provide liaison with colleagues in other sciences to attack problems which they have in common, *e.g.*, training and retraining, use of educational technology, low-cost instructional equipment, *etc.* (See also 1.7.3).
- 2.6.2 To press that those responsible for budgetary allocations should provide funds for educational research and development—about 5% of operating budget—and that the involvement of chemists in such research should be accorded equal status with other professional activities. (See also 3.9)

3. INDIVIDUAL INSTITUTIONS

- 3.1 Chemistry should play a significant part in general education and in education for citizenship and not just be a discipline for the instruction and training of chemists.
- 3.2 A precise statement of the objectives of chemical education should be made, and this should include objectives beyond those specifically concerned with factual knowledge and its immediate applications (See also 1.1.2). These objectives should be known to teachers and students, and the assessment should reflect the objectives.
- 3.3 The chemistry curriculum at undergraduate level should consist of a 'core' course followed by a variety of 'package' courses in (a) the chemical area, (b) scientific, nonchemical areas, and (c) non-

scientific areas (see 3.5), from which a student can choose a mixture for his graduation requirements to suit his personal abilities, interests, and intentions. Feedback about such programmes in existence, or under consideration, should be collated by national chemical education groups and then submitted to IUPAC. The 'core' course should be not less than one year in duration, should be at the professional level, should be more integrated with respect to subject matter than traditional courses, and should be designed and presented by the most effective and experienced teachers in a department.

- 3.4 Courses should be developed that are concerned with the larger and broader issues of chemistry, including integrated courses illustrating the relationship between natural sciences, technology, and economics, the needs of society and the social implications of science. (See 3.5)
- 3.5 During the first two years of an undergraduate course there should be 15-20% of the time available devoted to nonscientific studies, such as economics, sociopolitical studies, philosophy, and literature.
- 3.6 Chemistry students should spend a period of at least three months in industry during their university course—after 'basic studies' and before special options. In addition, the possibilities of introducing university students into school teaching, under supervision, should be explored.
- 3.7 The role that chemistry plays in industry should be clarified in order to inform students of the significance of industrial practices.
- 3.8 The opinions of students and young professionals about chemistry teaching and careers in chemistry should be obtained as an essential feedback in designing courses, and course objectives should include specific plans for influencing and changing behaviour of students.
- 3.9 Senior students should be involved in teaching whenever possible, and participation of students in research programmes should be encouraged at an early stage. (See also 2.6.2)
- 3.10 Educational institutions should encourage the judicious use of new methods of teacher training, including various aspects of modern educational technology in the teaching of chemistry. This will involve the adequate training of the teachers concerned in the new techniques.
- 3.11 The career structure of university chemistry teachers should give greater consideration to contributions to teaching and/or educational research. (See also 2.6.2)
- 3.12 Cooperation between industry and university and between universities should include exchange of personnel—internationally as well as within individual countries.

IUPAC PUBLICATIONS

1973

A compilation of IUPAC Publications in 1972 was published in *Information Bulletin* No. 45 (May 1973). The present listing attempts to cover everything issued during 1973.

The IUPAC Secretariat would be pleased to receive notification of any omissions from this listing, especially of translations completed or in process of being prepared of IUPAC nomenclature recommendations.

Pure and Applied Chemistry*

- Vol. 33, No. 1: Plenary Lectures from VIII International Symposium on Chemistry of Natural Products, New Delhi (India), February 1972
- Vol. 33, Nos. 2-3: Plenary Lectures from IV International Photochemistry Symposium, Baden-Baden (Germany), July 1972
- Section on Organic Coatings: Recommended Methods for Analysis of Alkyd Resins
- IUPAC-IUB Commission on Biochemical Nomenclature: Abbreviated Nomenclature of Synthetic Polypeptides (Polymerized Amino Acids)
- IUPAC-IUB Commission on Biochemical Nomenclature: Definitive Nomenclature for Vitamins B-6 and Related Compounds
- Vol. 33, No. 4: Plenary Lectures from XIV International Conference on Coordination Chemistry, Toronto (Canada), June 1972
- Commission on Molecular Structure and Spectroscopy: Tables of Wave-numbers for Calibration of Infrared Spectrometers—III and IV: 600—1 cm⁻¹
- Vol. 34, No. 1: Plenary Lectures from International Congress on Analytical Chemistry, Kyoto (Japan), April 1972
- Vol. 34, No. 2: Plenary and Main Lectures from International Symposium on Photochemical Processes in Polymer Chemistry, Leuven (Belgium), June 1972
- Vol. 34, Nos. 3-4: Plenary Lectures from International Symposium on Chemistry in Evolution and Systematics, Strasbourg (France), July 1972
- Vol. 35, No. 1: Plenary Lectures from III International Symposium on Carotenoids other than Vitamin A, Cluj (Romania), September 1972
- Vol. 35, No. 2: Plenary Lectures from International Symposium on Carbohydrate Chemistry, Madison (USA), August 1972
- Vol. 35, No. 3: Special Lectures from Symposium on Control of Mycotoxins, Göteborg (Sweden), August 1972
- Macromolecular Division Working Party on Structure and Properties of Commercial Polymers: A Collaborative Study of Dynamic, Mechanical, and Impact Properties of PVC-II
- Vol. 35, No. 4: Main Lectures from III International Symposium on Medicinal Chemistry, Milan (Italy), September 1972

*Official journal of IUPAC and additional publications of the Union are available from Butterworth & Co. (Publishers) Ltd., 88 Kingsway, London WC2B 6AB, UK.

Much of the material which appears in the journal is published shortly afterwards in book form.

- Vol. 36, Nos. 1-2: Main Lectures from X and XI Microsymposia on Macromolecules, Prague (Czechoslovakia), August-September 1972
 Commission on Molecular Structure and Spectroscopy: Recommendations for Presentation of Raman Spectra for Cataloging and Documentation in Permanent Data Collections
- Vol. 36, No. 3: Invited Lectures from I International Symposium on Advances in Microbial Engineering, Marianbad (Czechoslovakia), August-September 1972
- Vol. 36, No. 4: Plenary Lectures from International Symposium on Ion-Selective Electrodes, Cardiff (UK), April 1973

Information Bulletin*

- No. 45, May 1973
 No. 46, October 1973

Appendices on Tentative Nomenclature, Symbols, Units, and Standards

- No. 30, August 1973: Classification and Nomenclature of Electroanalytical Techniques (Commission on Electroanalytical Chemistry)
- No. 31, August 1973: Nomenclature of Organic Chemistry: Section D—Organic Compounds containing Elements which are not exclusively Carbon, Hydrogen, Oxygen, Nitrogen, Halogen, Sulfur, Selenium, and Tellurium (Commission on Nomenclature of Organic Chemistry and Commission on Nomenclature of Inorganic Chemistry)
- No. 32, August 1973: Nomenclature of Iron-Sulfur Proteins (IUPAC-IUB Commission on Biochemical Nomenclature)
- No. 33, August 1973: Nomenclature and Conventions for Reporting Mössbauer Spectroscopic Data (Commission on Physiochemical Symbols, Terminology, and Units and Commission on Molecular Structure and Spectroscopy)

Technical Reports Appendices

- No. 7, August 1973: A Survey of Some Recommended Methods for Identification and Determination of the Phenol Group (Commission on Analytical Reactions and Reagents)
- No. 8, August 1973: Recommended Method for Aflatoxins in Cocoa Beans (Commission on Trace Substances)

Miscellaneous

- || Fermentation Technology Today: Proceedings of IV International Fermentation Symposium, Kyoto (Japan), March 1972
- † Man-made Polymers in Papermaking: Proceedings of Symposium, Helsinki, June 1972
- § Macromolecular Chemistry—8: Plenary and Main Lectures from International Symposium on Macromolecules, Helsinki (Finland), July 1972

*Available from IUPAC Secretariat, Oxford.

||Available from Society of Fermentation Technology, Yamada-Kami, Suita-shi, Osaka, Japan.

†Available from Finnish Pulp and Paper Research Institute, Helsinki, Finland.

§Available from Butterworth & Co. (Publishers) Ltd., London.

- || Reactivity of Solids: Proceedings of VII International Symposium on Reactivity of Solids, Bristol (UK), July 1972
- ¶ Catalysis (Vols. I & II): Proceedings of V International Congress on Catalysis, Miami Beach, Florida (USA), August 1972
- ‡ Chemistry, Physical Chemistry and Applications of Surface Active Substances (Vols. I and II.1): Proceedings of VI International Congress on Surface Active Substances, Zürich (Switzerland), September 1972
- § Medicinal Chemistry: Special Contributions from III International Symposium on Medicinal Chemistry, Milan (Italy), September 1972
- ** Pore Structure and Properties of Materials (Parts I and II): Proceedings of International Symposium, Prague (Czechoslovakia), September 1973
- †† Enzyme Nomenclature: Recommendations (1972) of the International Union of Pure and Applied Chemistry and the International Union of Biochemistry
- § Standard Methods for Analysis of Oils, Fats, and Soaps: Second Supplement
- §§ Bulletin of Thermodynamics and Thermochemistry—No. 16, December 1973
- ||| Bibliography on High Temperature Chemistry and Physics of Materials:
 - Vol. 17, No. 1: January-March 1973
 - Vol. 17, No. 2: April-June 1973
 - Vol. 17, No. 3: July-September 1973
 - Vol. 17, No. 4: October-December 1973
- ¶¶ Japanese translation of Manual of Symbols and Terminology for Physicochemical Quantities and Units (1969)

|| Available from Chapman & Hall Ltd., London.

¶ Available from North-Holland Publishing Co., Amsterdam.

‡ Available from Carl Hanser Verlag, Munich.

§ Available from Butterworth & Co. (Publishers) Ltd., London.

** Available from Akademia, Prague.

†† Available from Elsevier Scientific Publishing Co., Amsterdam.

§§ Available from Publications Distribution Service, University of Michigan, 615 East University Avenue, Ann Arbor, Michigan 48106, USA.

||| Available from Dr. M. G. HOCKING, Department of Metallurgy, Imperial College of Science and Technology, London, SW7 2BP, UK.

¶¶ Available from Chemical Society of Japan, 1-5 Kanda-Surugadai, Chiyoda-ku, Tokyo 101, Japan.

FORTHCOMING IUPAC-SPONSORED SYMPOSIA

II INTERNATIONAL MEETING ON BORON CHEMISTRY

Leeds, 25-29 March 1974

The second IME BORON meeting will be held under the auspices of the Inorganic Chemistry Division of IUPAC and the Dalton and Industrial Divisions of the Chemical Society, London. It will be centred on Bodington Hall at the University of Leeds.

Scientific Programme

The main topics will be introduced by a series of plenary lectures. There will also be sessions devoted to contributed papers covering these topics and related areas. Each session will include discussion periods as appropriate. The principal speakers will be:

Boron Hydrides	R. SCHAEFFER (USA)
Carboranes	S. HERMANEK and J. PLESEK (Czechoslovakia)
	R. N. GRIMES (USA)
Metallo-Carboranes	M. F. HAWTHORNE (USA)
Organoboron Compounds	A. G. DAVIES (UK)
	B. M. MIKHAILOV (USSR)
Metal Borides	V. I. MATKOVICH (USA)
Technical Applications of Boron Compounds	R. THOMPSON (UK)

These papers will be published subsequently in the official journal of IUPAC, *Pure and Applied Chemistry*.

Secretariat

The Secretary of the Local Organizing Committee is:

Dr. B. S. THOMAS
School of Chemistry
University of Leeds
Leeds LS2 9JT, UK
Telephone: Leeds (0532) 31751

CONFERENCE ON LABORATORY INSTRUCTION IN CHEMISTRY

Troy, New York, 10-12 June 1974

The laboratory experience, as an integral part of chemical instruction, has been under critical examination in recent years to define more precisely the role of direct student experimentation and the format of the laboratory organization in view of the apparent demands in sophisticated equipment, student time, space, *etc.* These aspects of the student chemistry laboratory, especially as they may relate to the overall trends in chemical education, will be reviewed critically at this Conference.

Rensselaer Polytechnic Institute, under the sponsorship of IUPAC, will host the Conference as part of Rensselaer's 150th anniversary celebration in 1974. The format will be informal, and will provide opportunity for participants to evaluate past, present and future aspects of laboratory instruction, to examine direction and innovation, and to exchange views and experience on the subject.

The Conference will cover five major areas, each keynoted by a plenary lecturer:

The Integrated Laboratory in Chemistry	J. C. MARTIN (Urbana, Illinois)
The General Chemistry Laboratory	J. A. YOUNG (Auburn, Alabama)
The Computer in Laboratory Instruction	C. WILKINS (Lincoln, Nebraska)
Instructional Aids and Equipment	J. A. BELL (Boston, Massachusetts)
Laboratory Organization	W. T. LIPPINCOTT (Tucson, Arizona)

In addition to contributed papers, it is planned to include panel discussions and special interest workshops in the programme and there will be opportunities for more informal discussions. Bound copies of abstracts will be given to attendees at registration. Exhibits of instructional laboratory equipment will be on display in the Conference building, RPI's air-conditioned modern Communications Centre, which has facilities for closed circuit TV, 16-mm sound motion pictures, TV tapes, 8-mm film loops, 35-mm and lantern slide projection and overhead projection, as well as preparation areas and equipment for live demonstrations.

Secretariat

Further information, including details of registration and accommodation, may be obtained by writing to the Conference Chairman:

Prof. R. L. STRONG
Department of Chemistry
Rensselaer Polytechnic Institute
Troy, New York 12181, USA
Telephone: (518) 270 6442

IV INTERNATIONAL CONFERENCE ON NONAQUEOUS SOLUTIONS

Vienna, 10-12 July 1974

The Conference is being sponsored by IUPAC and organized by Verein Österreichischer Chemiker.

Scientific Programme

Advances in the chemistry in covalent liquids, molten salts, and liquified metals as solvents are within the scope of the Conference. Emphasis will be given to solute-solvent interactions, both in pure solvents and in solvent mixtures, and hence to the consideration of the structural and dynamic features of the solutions in relation to phenomenological properties. It is

not intended to duplicate the International Coordination Chemistry Conferences by discussing in great detail complex formation in a particular medium. Electrochemistry in the solutions will be included although this will be treated in more detail in an ISE-Conference which will probably take place in Austria in 1975.

About 100 contributed papers will be admitted for oral presentation. Three parallel sessions will be held. A time of 15 minutes will be available for presentation of each paper with an additional 5 minutes for discussion. Because it is anticipated that the number of offered papers may exceed the number that can be presented, a selection may be made if necessary.

The official language is English. Although there is no argument against the use of any other language, it is recommended that papers be presented in English. Translation facilities will not be available.

The plenary lectures will be as follows and they will be published in *Pure and Applied Chemistry*:

G. HILLS (UK) Recent Advances in Molten Salts as Reaction Media

H. HOFMANN (Germany) Mechanisms of Complex Formation in Non-aqueous Solutions

U. MAYER (Austria) Ionic Equilibria in Donor Solvents

A. I. POPOV (USA) Alkali Metal NMR and Vibrational Spectroscopic Studies on Solvates in Nonaqueous Solutions

J. B. SENIOR (Canada) Some Aspects of Chemistry in Strongly Acidic Solvents

Conference Bureau

The Conference Bureau will be located at the Conference Centre in the new Chemistry Building of the Technische Hochschule, Getreidemarkt 9, where all scientific sessions will take place. The Intropa Travel Agency, which will be responsible for hotel arrangements, guided tours, excursions, theatre tickets, exchange of traveller's cheques and of currency, will have an office at the same place. Meanwhile, please address all enquiries to:

Intropa Travel Agency
Kärntnerstrasse 38
A-1010 Vienna, Austria
Telephone: 0222 528501

Registration

Details of registration and other information may be obtained from the Conference Secretary:

Prof. H. SCHINDLBAUER
Verein Österreichischer Chemiker
Eschenbachgasse 9
A-1010 Vienna, Austria

INTERNATIONAL SYMPOSIUM ON MACROMOLECULES

Rio de Janeiro, 26-31 July 1974

The Brazilian Academy of Sciences, the National Research Council of

Brazil, and the Science and Technology Secretariat of Guanabara State are pleased to invite participation in the International Symposium on Macromolecules to be held in Rio de Janeiro, Guanabara, under the sponsorship of IUPAC.

Scientific Programme

Symposia will be held on topics to be selected from such important areas in science and technology as the following:

- 1—Solution and bulk properties of polymers
- 2—Polymer characterization methods
- 3—Homo- and copolymerization reactions
- 4—Photopolymerization
- 5—Chemical reactions on macromolecules
- 6—Evaluation of polymer properties
- 7—Advances in polymer technology
- 8—Natural polymers—reactions and technology
- 9—Advances in biopolymers and their synthetic models

Main lectures and contributed papers will be presented in four conference rooms, in simultaneous sessions of Polymer Chemistry, Polymer Physical Chemistry, Polymer Technology, and Biopolymers. It is planned to have three mornings and four afternoons for each of these sections. The formal Opening and Closing Sessions will be plenary functions, at which Sir HARRY MELVILLE and Prof. H. MARK, respectively, will speak. The meeting will be held in the new Congress Center of the Hotel Nacional-Rio.

The Organizing Committee, taking into consideration the enormous contribution that Prof. CARL S. MARVEL has given to the development of research in polymers worldwide, has decided to honour him during the Opening Session of the Symposium.

The following are among the invited lecturers who have already accepted formally:

Section A: Polymer Chemistry

- G. BUTLER (USA) Perspectives in Cyclopolymerization
M. FARINA (Italy) Inclusion Polymerization
C. G. OVERBERGER (USA) Reactivity of Polymers in Organic Reactions
L. PORRI (Italy) Diolefin Polymerization by Transition Metal Catalysts—Recent Developments
H. RINGSDORF (GFR) Structure and Properties of Pharmacologically Active Polymers
G. SMETS (Belgium) Photopolymerization and Photoresponsive Polymers
J. K. STILLE (USA) The Synthesis of Rigid Chain Polymers

Section B: Polymer Physical Chemistry

- H. BENOIT (France) Conformational Transitions in Polymers
F. BOVEY (USA) High Resolution Proton and Carbon-13 Studies of Biopolymer Systems
S. KRIMM (USA) IR Studies of Chain Organization in Crystalline Polyethylene
P. MEARES (UK) Selective Transport Processes in Polymers
G. V. SCHULZ (GFR) Determination of MW Distributions by Column Methods and the Relations between the Distributions and the Mechanisms of Polyreactions
M. SZWARC (USA) Trends in Living Polymers

Section C: Polymer Technology

- J. FONTAN (Spain) Copolycondensation: Relationship between Structure and Properties in New Polymers of High Thermal Stability
F. FOSTER (USA) Advances in Polyethylene Technology
M. LEWIN (Israel) Advances in Cellulose Technology
M. MORTON (USA) Advances in Rubber Technology
B. RÅNBY (Sweden) Creativity in Teaching and Research in Polymer Technology
I. V. YANNAS (USA) Molecular Interpretation of Deformation in Glassy Polymers

Section D: Biopolymers

- E. DAWES (UK) The Role and Regulation of Polyhydroxybutyrate as a Reserve in Microorganisms
G. KHORANA (USA) Total Synthesis of a Gene and the Problem of its Control Elements
G. MANECKE (GFR) Reactive Polymer Carriers and the Insolubilization of Enzymes
R. B. MERRIFIELD (USA) Solid Phase Protein Synthesis
H. G. PEREIRA (UK) Polymerization of Adenovirus Proteins
A. S. PERLIN (Canada) Structure of Sugars and Polysaccharides by NMR

Symposium Languages

The official language will be English, though papers may be presented either in English or in any of the following languages, for which there will be simultaneous translation into English: Portuguese, Spanish, Italian, French, and German.

Correspondence

Enquiries and other correspondence concerning the Symposium should be addressed to:

Prof. ELOISA BIASOTTO MANO
Simpósio Internacional de Macromoléculas
Academia Brasileira de Ciências
Caixa Postal 229
20.000 Rio de Janeiro, GB
Brazil

VII INTERNATIONAL SYMPOSIUM ON CARBOHYDRATE CHEMISTRY

Bratislava, 5-9 August 1974

Following the resolution of the International Steering Committee for Carbohydrate Chemistry at the meeting in Madison in 1972, the Institute of Chemistry of the Slovak Academy of Sciences is organizing the VII International Symposium on Carbohydrate Chemistry under the sponsorship of IUPAC.

Scientific Programme

The Symposium will provide an opportunity to present papers and discuss

recent research and developments in the following topics in carbohydrate chemistry and biochemistry:

Theoretical Studies

- (a) physical chemistry
- (b) organic chemistry
- (c) reaction mechanisms
- (d) stereochemistry

Plant and Wood Polysaccharides

- (a) plant gums
- (b) polyuronides
- (c) cellulose
- (d) hemicellulose
- (e) lignin-saccharide complexes

Biochemistry

- (a) enzymes of carbohydrate metabolism
- (b) structure and properties of biologically active complex saccharides
- (c) cell wall polymers

Plenary lectures will be presented as follows:

- N. K. KOCHETKOV (USSR) Pathways of Synthesis of Specific Polysaccharides
- W. G. OVEREND (UK) Some Approaches to the Synthesis of Amino-sugars and Branched-chain Sugars
- C. V. N. RAO (India) Immunochemical Approaches to the Structural Chemistry of Polysaccharides
- R. H. MARCHESSAULT (Canada) Influence of Acetate Groups on Carbohydrate and Polysaccharide Conformation in the Crystalline State
- CH. U. USMANOV (USSR) Physicochemical Investigations of the Structure of Cellulose Fibres
- J. BADDILEY (UK) Mechanism and Control of Cell Wall Synthesis in Bacteria
- J. MONTREUIL (France) Recent Data on the Structure of the Carbohydrate Moiety of Glycoconjugates: Metabolic and Biological Implications
- R. KOHN (Czechoslovakia) Ion Binding on Polyuronates
- D. HORTON (USA) Thio Sugars: Stereochemical Questions and Synthesis of Antimetabolites
- U. S. OVODOV (USSR) Structural Chemistry of Plant Glycuronoglycans

The plenary lectures delivered will be published subsequently in *Pure and Applied Chemistry*, official journal of IUPAC. Contributed papers will be presented in either English or Russian. No translation service will be available. All Symposium literature will be published in English.

General Information

Those wishing to register as a participant or requiring other information should write to:

VII International Symposium on Carbohydrate Chemistry
c/o Institute of Chemistry
Slovak Academy of Sciences
Dúbravská cesta
CS-809 33 Bratislava
Czechoslovakia

XVI INTERNATIONAL CONFERENCE ON COORDINATION CHEMISTRY

Dublin, 19-24 August 1974

The Conference will be held jointly at University College and Trinity College in Dublin, with the majority of the scientific meetings being held at University College.

The City is a well known tourist centre and is well provided with hotels covering a range of accommodation. In addition, student hostel accommodation will be available at Trinity College.

Scientific Programme

The Conference will be concerned with recent developments of coordination chemistry in the following fields:

- (1) Biological aspects of coordination chemistry
- (2) Physical methods and bonding
- (3) Inorganic reaction mechanisms
- (4) Reactions of coordinated ligands including catalysis
- (5) Coordination chemistry and the environment

Plenary lectures will be given by:

B. L. VALLEE (USA)	Functional and Conformational Properties of Metalloenzymes
C. BALLHAUSEN (Denmark)	On the Information Content in a Weakly Structured Absorption Band
H. TAUBE (USA)	Intramolecular Electron Transfer
J. LEWIS (UK)	Reactions of Olefins with some Group VIII Metal Carbonyls
A. E. MARTELL (USA)	Influence of Natural and Synthetic Ligands on the Transport and Function of Metal Ions in the Environment

and they will be published subsequently in the IUPAC journal, *Pure and Applied Chemistry*. In addition, some 15 session lectures of about 40 minutes duration will be given covering the main areas of the programme. Contributed papers will be of about 20 minutes duration.

The official language will be English. No arrangements will be made for simultaneous translation. Speakers in other languages are recommended to distribute a written text in English at the presentation of their contribution.

Secretariat

Please address correspondence to:

Dr. WILLIAM J. DAVIS
Secretary, XVI ICC
Chemical Laboratory
Trinity College
Dublin 2, Ireland

The official travel agent for the Conference, in respect of both travel and accommodation, is:

Martinstravel
Stillorgan Road
Dublin 4
Ireland

IV INTERNATIONAL CONFERENCE ON RAMAN SPECTROSCOPY

Brunswick, Maine, 26-30 August 1974

This Conference is the fourth of a series which began in Ottawa (1969), followed by Oxford (1970), and Reims (1972). It is cosponsored by IUPAC, the Optical Society of America, and the National Science Foundation. The programme will include the following topics:

I. General Session

- (1) Molecular Structures and Applications
- (2) Band and Line Profiles
Raman scattering
Rayleigh scattering
- (3) Large Angle Intramolecular Motions
Internal rotation, pseudo rotation, and large amplitude skeletal vibrations
- (4) Intensities in Gases, Liquids, and Solids

II. Nonlinear, Resonance and Electronic Raman Spectroscopy

- (1) Resonance Raman Scattering
- (2) Picosecond Spectroscopy
- (3) Electronic Raman Scattering

III. Solid State Raman Scattering

IV. Biological, Optically Active, and Polymer Molecules

V. Instrumentation and New Techniques

- (1) Ultramicro and Novel Sampling Techniques
- (2) Dye Lasers in Raman Spectroscopy
- (3) Mode Tunable Lasers
- (4) New Instrumentation and Data Processing
- (5) Rapid Scanning Raman Spectroscopy
- (6) Atmosphere and Water Pollution Studies
- (7) Flame and High Temperature Studies
- (8) Industrial Analytical Applications
- (9) Unstable Species and Matrix Isolation

VI. Post-Deadline Papers

Session VI has been tentatively included in the schedule in order to accommodate new and urgent results that are too significant to be bypassed because of the abstract deadline.

Presentations will be divided into three categories: invited lectures—an in depth summary of selected topics (40 min), invited papers—detailed presentations of current research topics (25 min), and contributed papers—brief descriptions of new results (13 min). Parallel sessions will be held during part of the Conference. Abstracts will be available on arrival at the meeting. The official language will be English.

Housing and Facilities

The Conference will be held at Bowdoin College. The campus is situated in the centre of Brunswick, Maine, about 25 miles northeast of Portland on Interstate Highway 95. Brunswick is on the shore of Casco Bay and is within

minutes to an hour from beach, lake, mountain, and wilderness regions. Accommodation and meals will be available on campus for participants and their guests for the duration of the meeting.

Meeting Correspondence

Please address all enquiries to the Secretary of the Organizing Committee:

Dr. JAMES E. GRIFFITHS
Bell Laboratories
Murray Hill, New Jersey 07974
USA
Telephone: (201) 582-3034

I INTERNATIONAL CONFERENCE ON ORGANIC SYNTHESIS

Louvain-la-Neuve, 26-30 August 1974

The Organic Chemistry Division of IUPAC has decided to launch a new series of biennial meetings devoted to Organic Synthesis. The first of these events, which will be held successively in the various member countries of the Union, will take place in Belgium on the new campus of the Catholic University at Louvain-la-Neuve.

The proceedings will be held daily in plenary session. Seminars on specific questions may be arranged on the spot. Following a questionnaire several subjects of the Conference have already been suggested: fundamental problems of organic synthesis such as planning, new general methods, physical activation, effect of the reaction medium, biomimetic synthesis, stereochemical control, industrial organic synthesis. The plenary lectures will be published in the official journal of IUPAC, *Pure and Applied Chemistry*.

Registration

The number of participants will be limited to approximately 200 persons. For further information, including full details of the scientific programme, accommodation, meals, excursions, *etc.*, please write to the Conference Secretariat:

Dr. L. VAN SIMAEYS
Place des Sciences 3
B-1348 Louvain-la-Neuve
Belgium

IV POLISH CONFERENCE ON ANALYTICAL CHEMISTRY

Warsaw, 26-31 August 1974

The meeting is being organized by the Commission of Analytical Chemistry of the Polish Academy of Sciences under the sponsorship of IUPAC.

Scientific Programme

The scope of the Conference will cover the broad field of analytical chemistry. However, trace analysis and organic analysis will be preferred subjects.

Besides short communications which will be selected from among the submitted papers on the basis of originality and contribution that they make to advancement of analytical chemistry, several plenary lectures by invited eminent speakers are to be given. The papers may be presented in Polish, English, Russian, French or German, although English and Russian will be preferred. The plenary lectures will be published in *Pure and Applied Chemistry*, the official journal of IUPAC. Other papers may appear in *Chemia Analityczna*.

Information

All correspondence should be addressed to the Secretary of the Organizing Committee:

Dr. R. DYBCYŃSKI
Institute of Nuclear Research
Ul. Dorodna 16
PL-03 195 Warsaw
Poland

XIV MICROSYMPOSIUM ON MACROMOLECULES: CROSSLINKING AND NETWORKS

Prague, 26-29 August 1974

Topics

- (1) Crosslinking reactions and crosslinking statistics
- (2) Network topology
- (3) Homogeneity and nonhomogeneity of networks
- (4) Network properties (mechanical, optical, and other)

Aim

Main lectures and short communications will be devoted mainly to discussions of the relationships between the formation, structure, and properties of networks. The contributions will not be confined to the network type—they may deal with nonpolar as well as hydrophilic or polyelectrolyte networks.

Topic (1) includes all types of crosslinking reaction, either equilibrium or kinetically controlled, and also the effect of structure of the starting monomers, and of reactivity of the functional groups; it concerns the pre- and postgelation stages of network formation, theoretical approaches to the treatment of cyclization reactions, diffusion control competition for space during branching and crosslinking, as well as the respective experimental results and methods of study. Topic (2), which is closely related to topic (1), is concentrated on the description of the composition and structure of the crosslinked system, e.g., distribution between the sol and the gel, concentration of elastically active chains, or the amount of trapped entanglements. In topic (3) detailed attention will be devoted to processes which may lead to the formation of nonhomogeneities induced either by the crosslinking itself or by an interaction of the forming network with the surrounding medium (phase separation, aggregation, cluster formation), and also to the experimental methods of investigation of nonhomogeneities. In topic (4)

will be contributions in which the study of mechanical, optical, and other physical properties may give information about the network structure, topology, and conformational behaviour of network chains. This topic involves contributions on rubber elasticity, swelling, or phase equilibria between the gel and the liquid phases.

About 8 or 9 main lectures will be presented at this Microsymposium. These will be published subsequently in *Pure and Applied Chemistry*, the official journal of IUPAC.

Secretariat

All enquiries should be directed for the attention of the Prague Meetings on Macromolecules Secretariat at:

Institute of Macromolecular Chemistry
Czechoslovak Academy of Sciences
Petřiny 1888, CS-162 06 Prague 616
Czechoslovakia

IV DISCUSSION CONFERENCE ON MACROMOLECULES: HETEROGENEITIES IN POLYMERS

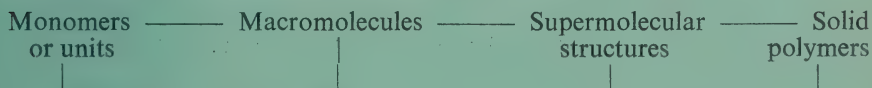
Marienbad, 2-5 September 1974

Topics

- (1) Heterogeneities in the molecular structure of polymers, their origin and consequences
- (2) Heterogeneities in the supermolecular structure of polymers, their origin and consequences
- (3) Heterogeneities in the macroscopic structure of polymers, their origin and consequences

Aim

The Discussion Conference will deal with heterogeneities which are defined on the one hand as (a) defects of the structure order at different levels, characterized as a rule as isolated nonhomogeneities or anomalies in otherwise homogeneous surroundings, and on the other as (b) products of ordering processes which lead to the formation of molecular, supermolecular, or macroscopic structures (domains) having different physical and/or physico-chemical properties. Thus, heterogeneities may arise at several levels, which also will be dealt with at the Conference with the objective of finding mutual relationships (if any) and formulating their general principles:



Heterogeneities may also be formed more or less spontaneously (natural heterogeneities) or intentionally (functional heterogeneities) without, however, any sharp boundary between them. Topics (1)-(3), which virtually involve the whole extent of possible heterogeneities, have rather a categorizational character. The concrete topics will be identical with the individual

subjects of each of the 10-12 invited lectures envisaged for the Conference; they will represent a selection of new unconventional problems or approaches, having fundamental character and will be published in *Pure and Applied Chemistry*. The discussion contributions will have the form of questions and comments on the lectures, or of a concise exposé of a related problem; in no case, however, will they be identical with the short communications describing in detail an isolated problem, but be preferably general (synthetic, if possible) problems covering the principles of the phenomena discussed.

The concrete topics (chosen as outlined above, which ensures an active participation of the top scientists in the conception of the Conference and the up-to-dateness of the problems discussed) will be announced later. It is quite justified to expect that not only the unconventional conception, but also the discussion character of the topics involved will be stressed (analysis of the problem, exposé of the viewpoints at issue and their confrontation, synthesis or generalization of the existing relations). The expected character of the topics follows from the conception of the discussion in the terms 'origin-heterogeneity-consequence'; several examples are given:

- (A) Molecular (supermolecular) heterogeneities and limiting physical properties of polymers (*e.g.*, theoretical strength, maximum toughness, thermal endurance, thermal and electric conductivity, transparency and other optical properties, *etc.*)
- (B) Thermodynamic causes of the formation and existence of heterogeneities, ordering phenomena
- (C) Heterogeneities and energy propagation in polymers
- (D) Molecular (supermolecular) heterogeneities and memory phenomena
- (E) Heterogeneities and transport phenomena in polymers
- (F) Heterogeneities and sorption effects in polymers
- (G) Molecular heterogeneities and association of macromolecules

It can be seen from the above examples that the main attention will be devoted to the physical and physicochemical consequences of heterogeneities, irrespective of the chemical or physical nature of their cause. The purely morphological aspects of the discussion of heterogeneities will be confined to the extent necessary for understanding the mechanism of their formation and the character of the resulting properties. Also, problems connected with gels and polymer networks (including branching) will be restricted to those which document the rather general aspects of heterogeneities, in view of the fact that the problems of gels and polymer networks will be dealt with in two other meetings in 1974 (Discussions of the Faraday Society and the XIV Prague Microsymposium).

Secretariat

All enquiries should be directed for the attention of the Prague Meetings on Macromolecules Secretariat at:

Institute of Macromolecular Chemistry
Czechoslovak Academy of Sciences
Petržiny 1888, CS-162 06 Prague 616
Czechoslovakia

INTERNATIONAL SYMPOSIUM ON MACROMOLECULES

Madrid, 15-20 September 1974

The meeting is being organized by the Instituto de Plásticos y Caucho, CSIC (National Council of Scientific Research). It will be held at the Palacio de Congresos, Avenida del Generalísimo 29, Madrid. This new building houses ten auditoria for lectures, discussion rooms, and various offices and services for the Symposium such as travel bureau, exchange and bank services, post office, restaurants, *etc.*

Programme

The scientific programme will be divided into the following four sections:

- (1) New developments in polymerization
- (2) Chemical modifications and reactions on polymers
- (3) Properties in amorphous and crystalline polymers
- (4) Influence of structure on technical properties

Main Lectures will be given as a separate series. The following speakers have already accepted:

P. J. FLORY (USA)	Molecular Theory of Rubber Elasticity
H. BENOIT (France)	Application of Neutron Scattering to the Problem of Configurations of Polymers in Bulk
G. SMETS (Belgium)	Photochemical Reactions in Polymeric Systems
J. FURUKAWA (Japan)	Mechanism of Diene Polymerization

These papers will subsequently be published in the IUPAC journal, *Pure and Applied Chemistry*. Invited and Symposium Lectures will be given during the meeting. The number and sections where they will take place will be notified later. Short communications will also be presented.

There will be an opportunity during the Symposium for the presentation and discussion of two reports from the IUPAC Working Party on Structure and Properties of Commercial Polymers: Relationship between Basic Parameters, Melt Rheology, Processing, and End-use Properties of Three Samples of Low Density Polyethylene [prepared by J. MEISSNER (GFR)].

Determination of Rheological Properties of a Polyvinyl Chloride Compound [prepared by J. L. S. WALES (Netherlands)].

Symposium Languages

The main lectures will be given in English. Contributed papers may be presented in any language, but the organizers suggest that speakers should use preferably English or French that is commonly understood by most participants. Simultaneous translation will not be arranged.

Correspondence

Enquiries and other correspondence concerning the Symposium should be addressed to:

Prof. J. G. FATOU, General Secretary
International Symposium on Macromolecules
c/o Instituto de Plásticos y Caucho
Juan de la Cierva 3,
Madrid-6, Spain

XXV IUPAC CONGRESS

Jerusalem, 6-11 July 1975

The Congress will be held at the Jerusalem Convention Center (Binyanei Ha'ooma) under the auspices of His Excellency, The President of the State of Israel, Prof. EPHRAIM KATZIR, and under the sponsorship of the Israel Academy of Sciences and Humanities, the National Council for Research and Development, and the Hebrew University of Jerusalem.

Tentative Scientific Programme: Main Topics

- A. *Organic Chemistry*
 - (1) New theoretical insights into organic molecules
 - (2) Chemistry of excited states
 - (3) Novel instrumental methods of structure determination
 - (4) Computers in organic synthesis and structure determination
 - (5) Novel synthetic applications of organometallic compounds
 - (6) Ylid chemistry
 - (7) Prebiotic chemistry and organic geochemistry
 - (8) Approaches to the structure of biological receptors
 - (9) Stereochemical aspects of biogenesis
- B. *Physical Chemistry*
 - (1) Condensed phases
 - (2) Lasers in chemistry
 - (3) Molecular spectroscopy
 - (4) Molecular dynamics
 - (5) Interfacial electrochemistry
 - (6) Molecular structure
 - (7) Molecular conformations
 - (8) Symposium on 50 years of quantum chemistry
- C. *Medicinal Chemistry*
 - (1) Prostaglandins
 - (2) Chemistry and biochemistry of ageing
 - (3) Chemistry of memory
 - (4) Chemistry of pain relief
 - (5) Chemotherapy of tropical diseases
 - (6) Molecular pharmacology
 - (7) Drugs and toxins from marine sources
 - (8) Histochemistry
 - (9) Immunosuppression
- D. *Applied Chemistry*
 - (1) Processes for future chemical industries
 - (2) Chemical aspects of future energy sources
 - (3) Food resources through chemistry
 - (4) Surface chemistry and surface activity
 - (5) Chemical processes for water desalination
 - (6) Industrial use of water
 - (7) Recycling and reuse of wastes
 - (8) Chemical means for reduction of environmental pollution

The following Symposium will be held jointly with the Division of Macromolecular Chemistry of IUPAC, in the week following the Congress:

E. *Macromolecular Chemistry*

III Aharon Katzir-Katchalsky Conference

- (1) Developments in polymer theory
- (2) Surface- and electrochemistry of macromolecules
- (3) Ions in polymeric systems
- (4) Polymeric reagents
- (5) Membranes—synthesis and function
- (6) Biomedical applications of macromolecules
- (7) Specialized polymeric systems in structural materials
- (8) Polymers in pollution abatement

The official language of the Congress is English. Papers may be presented in any language, but the use of a widely understood one is recommended.

General Information

The weather in Jerusalem in July is pleasantly warm during the day and cool in the evenings.

Peltours Ltd. are the official travel agents and will provide all the necessary services to participants. Their offices and agents abroad will offer the best possible travel arrangements to and from Israel. In Israel, *Peltours* will be responsible for hotel accommodation, meet participants on arrival in Israel, arrange transfer to hotels, and provide all the sightseeing programmes.

El Al Israel Airlines are the official carriers and their offices throughout the world will be at the service of participants in connexion with flight arrangements.

Further information on the Congress may be obtained by writing to:

Organizing Committee
XXV IUPAC Congress
POB 16271, Tel Aviv
Israel

THE ENVIRONMENT

A detailed account of the purposes, structure, and activities of the ICSU Scientific Committee on Problems of the Environment (SCOPE) appeared in *Information Bulletin* No. 46 (October 1973, pp. 4-14). A third Report has recently been issued by SCOPE (for details of the earlier Reports see *Inf. Bull.* No. 45, May 1973, p. 91):

Global Environmental Monitoring System: Action Plan for Phase I—R. E. MUNN, Consultant appointed by SCOPE to the UN Inter-Agency Working Group on Monitoring, Co-Chairman of SCOPE Commission on Environmental Monitoring and Assessment—1973, 130 pp., \$3.00

Copies are available from:

Mr. H. A. W. SOUTON
Executive Secretary of SCOPE
c/o Royal Society
6 Carlton House Terrace
London SW1Y 5AG, UK

RECOMMENDATIONS OF II MEETING OF ICSU GENERAL COMMITTEE*

Leningrad, 19-21 September 1973

THE GENERAL COMMITTEE OF ICSU:

Cooperation in Marine Research

Recognizing the need for improved understanding of the marine biota, their productivity, and their reaction to changes in the environment, both natural and manmade, particularly to allow the maximum sensible use of the living resources of the ocean;

Realizing that close international and interdisciplinary collaboration is needed to elucidate the interlocking biological and physicochemical problems of the ocean;

Notes with appreciation the leading part played by SCOR, in cooperation with IOC, FAO, UNESCO, and regional bodies, in stimulating and coordinating work in this field;

Invites all ICSU bodies concerned with the ocean and the atmosphere to cooperate with SCOR in this work; and

Further invites SCOR to report progress in this field to the XV General Assembly of ICSU (1974).

Cooperation in Water Research, Nonmarine

Recognizing that interest in, research on, and development of water resources is increasing rapidly throughout the world, and especially in developing countries, and that a number of organizations are active in this field, sometimes without full knowledge of each other's spheres of interest;

Recommends that the President of ICSU should invite representatives of the organizations concerned to a meeting designed to describe and outline their spheres of interest and programmes of activity.

Cooperation in Studies of Planetary Systems

Wishing to avoid unnecessary overlap between the scientific activities of its member organizations;

Stressing the importance of close cooperation and coordination in fields where overlap might occur;

Invites the organizations actively interested in problems of planetary systems to investigate, in mutual cooperation, how such overlap could be reduced; and

Requests these organizations to report on this matter to the XV General Assembly of ICSU.

SCOPE

Invites all ICSU National Members to establish committees for SCOPE where these do not exist and to formulate proposals concerning environmental problems which require an international and interdisciplinary approach.

*The official representative of IUPAC to the meeting in Leningrad was Prof. J. BÉNARD (France). He has now been succeeded as the official representative of IUPAC to the ICSU General Committee by Prof. Sir HAROLD THOMPSON (UK).

Global Atmospheric Research Programme

Recalling the approval by the XIV General Assembly of ICSU of the findings and recommendations of the joint ICSU-WMO Planning Conference on the First GARP Global Experiment (FGGE) held in Geneva, 5-8 September 1973,

Noting the report of the Study Panel on Institutional Arrangements for FGGE appointed by the Secretary General of WMO in conjunction with the Secretary General of ICSU;

Concurs with the recommendation of that Panel that 'a central policy and coordinating body for FGGE be established which should be an inter-governmental Panel of the WMO Executive Committee';

Concurs with the recommendations of the Panel that 'the JOC would be the principal scientific advisory body' for the detailed planning and implementation of FGGE;

Concurs with the recommendation that 'FGGE Project Office be established as part of the WMO Secretariat and that it should be headed by a Director of FGGE (D/FGGE)';

Approves the suggestion that the Director of FGGE (D/FGGE) would be responsible to the Secretary General of WMO and as D/JPS to the JOC';

Concurs with the resolution of the Executive Board of ICSU that the scientific integrity of this complex international experiment will be most effectively maintained by combining the post of D/FGGE with that of D/JPS.

Importance of Fundamental Research

Being aware of the importance of fundamental scientific research for the solution of environmental problems;

Being further aware of the importance of such research for the cultural and economic progress of developing countries;

Asks the ICSU scientific organizations to make due mention of (i) fundamental research as a general basis for future applications of science in their reports to ICSU as well as (ii) their contribution to the furtherance of scientific research in developing countries.

Registration Fees for Meetings, Symposia, Congresses

Recommends that for international symposia, congresses, and other meetings sponsored by members of the ICSU family, the registration fee, that is the right to attend the meeting, should not exceed US \$30;

Recommends further that under no circumstances should it exceed US \$50.

Coordination of Scientific Meetings

Wishing to avoid, when possible, unnecessary duplication in scientific meetings organized by the scientific organizations in ICSU;

Requests that all members of the ICSU family send information on symposia and colloquia under consideration to the ICSU Secretariat; and

Asks the ICSU Secretariat to distribute such information among members of the ICSU family as early as possible.

Reports of ICSU's Adhering Scientific Organizations

Noting that the actual Reports of the scientific bodies often pay too little attention to scientific research as compared to administrative matters;

Wishes to be informed in sufficient detail about the large scientific projects being undertaken by the scientific organizations in ICSU;

Urges these organizations to report adequately on such projects in their Reports to ICSU, in particular drawing attention to the scientific significance and scope of the projects, their estimated time-scale, development, and expected termination date, and other information such as the degree of international and interdisciplinary involvement.

Newsletters

Noting the need to inform individual scientists about the activities of ICSU, *Recommends* that the Newsletters and similar publications of the members of the ICSU family should in the future publish items of news concerning activities of other members which might be of interest to the readers;

Requests the Unions, Committees, Commissions, and Permanent Services to transmit items of information several times a year to the Editors of the Newsletters of other bodies whose members might be interested. Such items should include an address from which additional information can be obtained. The ICSU Secretariat is available to act as a clearing house for those items of information if required.

Public Relations

In view of the fact that both the scientific and nonscientific sectors of the community are inadequately informed about the work of ICSU;

Requests

- (i) the Executive Board to prepare a public relations programme to inform the world scientific community and the general public of the nature and value of ICSU's work, and

Invites National Members to cooperate;

- (ii) the Scientific Unions to inform through their national adhering organizations and through other appropriate channels the scientific and general academic communities, industry, and if possible, relevant government departments of the nature and value of their work.

Relations with Other Organizations

In view of the progressive increase in the interdisciplinary character of scientific research and the proliferation, outside the ICSU family, of international organizations concerned with specific topics,

Recommends that:

- (i) the Secretary General invite the Scientific Unions to examine their programmes with the object of exposing those of possible interdisciplinary character and to take the initiative in establishing appropriate inter-union liaison at the working level;
- (ii) in each Union, formal liaison should be actively promoted, by association or affiliation, with non-ICSU bodies whose interests are closely related to its own so that conflicts of interest can be avoided, and that the ICSU Secretariat be kept informed of these actions.

ICSU Secretariat
51 Boulevard de Montmorency
F-75016 Paris, France

ICSU ABSTRACTING BOARD*

The Board has recently issued a statement to indicate its position on the subject of

Repackaging versus Duplication

Changing emphases in science and technology are leading to the initiation of secondary information services designed to help with the solution of problems which often involve several disciplines or are interdisciplinary in character.

Despite international activities (UNISIST Recommendation 8, 1971; ICSU AB, and others) devoted to cooperation and to avoiding duplication wherever feasible, the newly emerging services frequently develop separately and independently data bases which do little more than duplicate the material already being processed and accumulated in the major data bases of the already existing secondary services in science and technology.

The Member Services of the ICSU AB, which involve all scientific and technological disciplines, process among them more than three million references to the primary literature each year. Within these three million there is duplication, some because secondary services may cover the science literature in different languages, but steps are being undertaken at the input level of a worldwide system for abstracting and indexing services to reduce duplication as much as possible.

A compilation or repackaging from the existing resources would usually meet most of the requirement of the new services without risk of further duplication. These services then would be in a position to concentrate on improving the effectiveness in dissemination of the abstracted and indexed information, and to expand their coverage by filling any gaps or omissions among the contributing services.

ICSU AB therefore recommends that every opportunity be taken to make use of the output of the existing secondary services to help meet new informational needs. The effect of such arrangements would be substantial savings in labour, time, and money overall, as well as more efficient use of the experience, extending over many years, which has been developed in the major secondary services.

The talents and resources of ICSU AB are available to assist in any advisory, consulting, or analytical role which may be desirable to help avoid duplication in abstracting and indexing on a national or international basis:

ICSU Abstracting Board Secretariat
17 Rue Mirabeau
F-75016 Paris, France

*The ICSU AB was established in 1953 for the purposes of organizing and promoting internationally the exchange and dissemination of information by secondary processing services in science and technology, and to deal with matters related thereto. The present representative of IUPAC is Dr. J. W. BARRETT (UK).

IV INTERNATIONAL CODATA CONFERENCE

Yerevan, 24-27 June 1974

The next in the biennial series of Conferences of the ICSU Committee on Data for Science and Technology (CODATA)* will take place in the high altitude Olympic training camp 'Tsachkadzor'. The camp is located near Yerevan, capital of the Armenian Republic, USSR.

This Conference will provide opportunities for the interchange of information and ideas on CODATA concerns, and for the establishment of closer scientific contacts among scientists from different countries, throughout the broad scope of disciplines embraced within CODATA.

Programme

The programme will include the *modus operandi* of both discipline- and mission-oriented data centres, their interaction and cooperation with data producers and users; computer usage in data systems organization; CODATA's role in meeting data needs for the geo-, cosmic-, and bio-sciences; progress in data handling for atomic, molecular, spectroscopic, and thermophysical data, *etc.*

Opportunities for discussion will be provided both in the main sessions and in the Task Group meetings. Whereas languages recognized by ICSU will be acceptable, the use of English is recommended both for oral presentations and for written texts submitted for publication in the Proceedings of the Conference.

Participation

Those persons wishing to receive information about participation in the Conference should write to the General Secretary:

Prof. E. F. WESTRUM, JR.
Department of Chemistry
University of Michigan
Ann Arbor, Michigan 48104
USA

Telephone: (313) 764 7357

The CODATA Central Office in Frankfurt was closed down in January 1974 and has been relocated at the same address as the ICSU Secretariat in Paris.

*CODATA was established by ICSU in 1966 to promote and encourage, on a world-wide basis, the production and distribution of compendia and other forms of collection of critically selected numerical and other quantitatively expressed values of properties of substances of importance and interest to science and technology. The present representative of IUPAC is Prof. W. KLEMM (GFR).

NOMENCLATURE, SYMBOLS, UNITS, AND STANDARDS

One of the main functions of the International Union of Pure and Applied Chemistry (IUPAC), carried out through the voluntary help and expertise of the Members of its Commissions, is to propose and get agreement on nomenclature, symbols, units, and standards. During recent years, this has become increasingly important, on the one hand because the range of chemistry has widened and it has become more relevant to other scientific fields; and on the other, because the rapid growth of chemistry demands quicker agreement about these matters. Often, Commissions of IUPAC work together with Commissions of other International Scientific Unions in preparing the recommendations.

In the past, recommendations of a scientific nature and relating to the establishment of international scientific usage (nomenclature, symbols, standards, *etc.*) were regarded as 'provisional'. National Adhering Organizations of IUPAC and individual specialists everywhere were asked to comment within eight months so that critical observations could be considered by the Commission or other body concerned. The recommendations, amended as seemed desirable, were then submitted for approval by the Council of IUPAC.

During recent years, the Union has issued the provisional recommendations as 'Appendices on Tentative Nomenclature, Symbols, Units, and Standards' to the IUPAC *Information Bulletin*. The final ('definitive') recommendations have been published subsequently in *Pure and Applied Chemistry*, the journal of IUPAC.

The Bureau of IUPAC has now decided that:

(i) Nomenclature previously issued by IUPAC as 'tentative' shall be termed 'provisional rules X' (X being the year of issue);

(ii) Symbols and units previously issued by IUPAC as 'tentative' shall be termed 'provisional recommendations X' (X being the year of issue);

(iii) Nomenclature previously issued by IUPAC as 'definitive' or 'final' shall be termed 'rules approved X' (X being the year of issue);

(iv) Symbols and units previously issued by IUPAC as 'definitive' or 'final' shall be termed 'recommendations approved X' (X being the year of issue).

The material will be published by IUPAC in the same two places as hitherto, taking into account the above changes of designation.

H. W. THOMPSON
President

FORTHCOMING APPENDICES TO IUPAC INFORMATION BULLETIN

The following Appendices are expected to appear soon

Appendices on Provisional Nomenclature, Symbols, Units, and Standards

Recommendations on Usage of the Terms 'Equivalent' and 'Normal' (Commission on Analytical Nomenclature)

Nomenclature of Tocopherols and Related Compounds (IUPAC-IUB Commission on Biochemical Nomenclature)

Nomenclature of Corrinoids (IUPAC-IUB Commission on Biochemical Nomenclature)

Recommendations for Presentation of NMR Data for Publication in Chemical Journals—B: Conventions Relating to Spectra from Other Nuclei (Commission on Molecular Structure and Spectroscopy)

Recommendations for Nomenclature and Spectra Presentation in Chemical Electron Spectroscopy Resulting from Excitation by Photons (Commission on Molecular Structure and Spectroscopy)

Definitions, Terminology, and Symbols in Colloid and Surface Chemistry—II: Heterogeneous Catalysis (Commission on Colloid and Surface Chemistry)

Technical Reports

Collaborative Study of the Determination of Aflatoxin M_1 in Milk (Section on Food)

Recommended Method for Aflatoxin in Copra, Copra Meal, and Coconut (Section on Food)

Development of a Method to Evaluate Sampling Plans Used to Estimate Aflatoxin Concentrations in Lots of Shelled Peanuts (Section on Food)

Proposed Guidelines for Testing of Single Cell Protein Destined as Major Protein Source for Animal Feed (Section on Fermentation)

Report on International Education of Medicinal Chemists (Section on Medicinal Chemistry)

Subscribers to the *Information Bulletin* receive all Appendices automatically and free-of-charge on publication.

SPECIAL EVENTS

VAN'T HOFF CENTENARY COMMEMORATION LEIDEN, 3 MAY 1974

In September 1974 a century will have elapsed since VAN'T HOFF published his famous paper:

'Voorstel tot uitbreiding der tegenwoordig in de scheikunde gebruikte structuur formules in de ruimte; benevens een daarmee samenhangende opmerking omtrent het verband tusschen optisch actief vermogen en chemische constitutie van organische verbindingen'

(A suggestion on the extension into space of the structural formulae at present used in chemistry; a note on the relation between the optical activity and the chemical constitution of organic compounds)

To celebrate this outstanding scientific event the Royal Netherlands Academy of Sciences (Van't Hoff Committee) and the Royal Netherlands Chemical Society (Division of Organic Chemistry) plan to organize a Commemoration, intended primarily to show the impact of the VAN'T HOFF-LE BEL concept of molecular three-dimensionality on present-day chemistry.

The celebration will be held in the Gorlaeus Laboratories, University of Leiden, Netherlands, following the II IUPAC Conference on Physical Organic Chemistry at Noordwijkerhout (29 April-2 May 1974).

Applications, enquiries and other correspondence concerning the Commemoration should be addressed to:

Dr. H. J. C. JACOBS
Gorlaeus Laboratories, University of Leiden
POB 75, Leiden, Netherlands

CENTENARY CELEBRATIONS OF SOCIETY FOR ANALYTICAL CHEMISTRY (SAC)

London, 16-19 July 1974

The Centenary Lecture

H. M. N. H. IRVING One Hundred Years of Developments in Analytical Chemistry

will be given after the Opening Ceremony and Presentation of Fraternal Greetings at the Royal Institution in Albermarle Street. Plenary lectures will be delivered on the following three days by

R. BELCHER	Analytical Chemistry and Education
C. WHALLEY	Analytical Chemistry in Industry
J. MARKLAND	Analytical Chemistry in Public Service

On each of the four days, at Imperial College of Science and Technology, there will be three simultaneous lecture streams in various subject divisions, with internationally known keynote lecturers participating.

Further details and registration forms may be obtained from:

The Secretary
Society for Analytical Chemistry
9-10 Savile Row
London W1X 1AF, UK

RECOMMENDED METHODS FOR THE ANALYSIS OF ALKYD RESINS

This is the second publication of the Subcommittee on Analytical Methods of the Organic Coatings Section of IUPAC, the first being 'Recommended Methods for the Analysis of Drying Oils' [*Pure Appl. Chem.* **10** (3), 189-238 (1965)]. The trend of the organic coatings industry has been to use oil-modified resins, particularly alkyd resins, in place of the simpler drying oils and this has brought the need for standard methods for analysis of these resins. The methods chosen for investigation were those considered to be of most importance in current practice:

Acid value, Saponification value, Hydroxyl value, Phthalic anhydride value, Fatty acids content, Identification of type of alkyd resin by infrared spectroscopy, Qualitative analysis of carboxylic acids in alkyd resins by gas chromatography, Identification and semi-quantitative determination of polyols in alkyd resins by gas chromatography

Of the chemical methods, particular attention has been given to the method for the determination of hydroxyl value, on which there were conflicting views. In a cooperative exercise, laboratories in five countries obtained highly satisfactory results by two methods and because there was little to choose between them both are included.

As envisaged in the earlier publication, increasing use is made of instrumental (chromatographic and spectroscopic) methods. In the present state of development they are of main value for qualitative or semi-quantitative analysis. The gas chromatographic methods were the subject of a further cooperative investigation involving laboratories in five countries.

The methods for the determination of phthalic anhydride content and fatty acids content are essentially equivalent to those of ASTM D563-52 and D1398-58, respectively.

Published in *Pure and Applied Chemistry* (Vol. 33, Nos. 2-3, 1973) and available as a reprint (26 pages) from the IUPAC Secretariat, price US \$0.75 (£0.25)—cash with order, postage free.

IUPAC COLLEAGUES DECEASED

We have been informed of the death of:

Canada Dr. H. HURTIG (13 December 1973)—Section on Pesticides (1961-), Commission on Terminal Pesticide Residues (1965-1973), Commission on Pesticide Residue Analysis (1965-1971)

UK Sir CHARLES DODDS (16 December 1973)—Treasurer of IUPAC (1957-1963), President of Division of Biological Chemistry (1951-1955)

USA Mr. R. T. O'CONNOR (1 December 1973)—Commission on Soaps and Oleochemicals (1973-)

CALENDAR OF IUPAC-SPONSORED MEETINGS

1974

March 24-29	IV International Conference on Crystal Growth (Conference Secretariat, Organizing Committee of ICCG-IV, Science Council of Japan, 7-22-34 Roppongi, Minato-ku, Tokyo 106, Japan)	Tokyo (Japan)
March 25-29	II International Meeting on Boron Chemistry (Dr. B. S. THOMAS, Secretary of Local Organizing Committee, II IME BORON, c/o School of Chemistry, University of Leeds, Leeds LS2 9JT, UK)	Leeds (UK)
April 29- May 2	II IUPAC Conference on Physical Organic Chemistry (Prof. TH. J. DE BOER, II IUPAC Conference on Physical Organic Chemistry, c/o Laboratorium voor Organische Scheikunde, Universiteit van Amsterdam, Nieuwe Achtergracht 129, Amsterdam, Netherlands)	Noordwijkerhout (Netherlands)
June 10-12	Conference on Laboratory Instruction in Chemistry (Prof. R. L. STRONG, Department of Chemistry, Rensselaer Polytechnic Institute, Troy, New York 12181, USA)	Troy/ New York (USA)
June 24-28	IX International Symposium on Chemistry of Natural Products (M. K. WARD, Executive Secretary, IX International Symposium on Chemistry of Natural Products, c/o National Research Council of Canada, Ottawa, Ontario K1A 0R6, Canada)	Ottawa (Canada)
July 3-9	III International Pesticide Chemistry Congress (Dr. J. LARINKARI, Chairman of Organizing Committee, III International Pesticide Chemistry Congress, POB 28, SF-00131 Helsinki 13, Finland)	Helsinki (Finland)
July 10-12	IV International Conference on Nonaqueous Solvents (Dr. H. SCHINDLBAUER, IV ICNAS, c/o Verein Österreichischer Chemiker, Eschenbachgasse 9, A-1010 Wien, Austria)	Vienna (Austria)
July 23-24	II International Symposium on Mycotoxins in Food (Prof. T. JUSZKIEWICZ, Instytut Weterynarii, Partyzantów 57, PL-24 100 Pulawy, Poland)	Pulawy (Poland)
July 26-31	International Symposium on Macromolecules (Prof. E. B. MANO, Simpósio Internacional de Macromoléculas, c/o Academia Brasileira de Ciências, Caixa Postal 229, 20.000 Rio de Janeiro, GB, Brazil)	Rio de Janeiro (Brazil)
August 5-9	VII International Symposium on Carbohydrate Chemistry (Dr. S. BAUER, Chairman of Organizing Committee, VII International Symposium on Carbohydrate Chemistry, c/o Institute of Chemistry, Slovak Academy of Sciences, Dúbravská cesta, CS-809 33 Bratislava, Czechoslovakia)	Bratislava (Czechoslovakia)
August 19-24	XVI International Conference on Coordination Chemistry (Dr. W. J. DAVIS, Secretary of Organizing Committee, XVI-ICCC, c/o Department of Chemistry, Trinity College, University of Dublin, Dublin 2, Ireland)	Dublin (Ireland)
August 26-29	XIV Prague Microsymposium on Macromolecules: Crosslinking and Networks (PMM Secretariat, c/o Institute of Macromolecular Chemistry, Czechoslovak Academy of Sciences, Petřiny 1888, CS-162 06 Praha 616, Czechoslovakia)	Prague (Czechoslovakia)

August 26-30	IV International Conference on Raman Spectroscopy (Dr. J. E. GRIFFITHS, Secretary of Organizing Committee, IV International Conference on Raman Spectroscopy, c/o Bell Laboratories, Murray Hill, New Jersey 07974, USA)	Brunswick/ Maine (USA)
August 26-30	I International Conference on Organic Synthesis (Secretariat of I International Conference on Organic Synthesis, Dr. L. VAN SIMAEYS, Place des Sciences 3, B-1348 Louvain-la-Neuve, Belgium)	Louvain-la-Neuve (Belgium)
August 26-31	IV Polish Conference on Analytical Chemistry (Dr. R. DYBCZYNSKI, Secretary of Organizing Committee, IV Polish Conference on Analytical Chemistry, c/o Institute of Nuclear Research, Ul. Dorodna 16, PL-03 195 Warszawa, Poland)	Warsaw (Poland)
September 2-5	IV Discussion Conference on Macromolecules (PMM Secretariat, c/o Institute of Macromolecular Chemistry, Czechoslovak Academy of Sciences, Petřiny 1888, CS-162 06 Praha 616, Czechoslovakia)	Marienbad (Czechoslovakia)
September 2-6	Biopolymer Interactions: Workshop on Physical Chemistry of Biologically Active Assemblies (Prof. A. RÖRSCH, Secretary of Organizing Committee, Biopolymer Interactions Workshop, c/o Laboratory of Biochemistry, Rijksuniversiteit Leiden, Wassenaarseweg 64, Leiden, Netherlands)	Amsterdam (Netherlands)
September 9-13	IV International Symposium on Medicinal Chemistry (Secretariat, IV International Symposium on Medicinal Chemistry c/o Merck Sharp & Dohme NV, Professional & Government Liaison, Waarderweg 39, POB 581, Haalem, Netherlands)	Noordwijkerhout (Netherlands)
September 10-14	II Symposium on Inorganic Phosphorus Compounds (Secretariat, II Symposium on Inorganic Phosphorus Compounds, c/o Department of Inorganic Chemistry, Prague Institute of Chemical Technology, Suchbátarova 5, CS-166 28 Praha-Dejvice, Czechoslovakia)	Prague (Czechoslovakia)
September 15-20	International Symposium on Macromolecules (Prof. J. G. FATOU, General Secretary of International Symposium on Macromolecules, Instituto de Plásticos y Caucho, c/o Juan de la Cierva No. 3, Madrid 6, Spain)	Madrid (Spain)
September 16-21	V International Conference of Organic Phosphorus Chemistry (Dr. M. MIKOLAJCZYK, V International Conference of Organic Phosphorus Chemistry, c/o Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences, Ul. Przedzalniana 72, Lodz, Poland)	Gdańsk (Poland)
September 23-27	II International Symposium on Chemistry of Non-benzenoid Aromatic Compounds (Dr. W. FRITSCH, General Secretary of Organizing Committee, II International Symposium on Chemistry of Nonbenzenoid Aromatic Compounds, c/o Gesellschaft Deutscher Chemiker, Postfach 900440, D-6000 Frankfurt 90, German Federal Republic)	Lindau (German Federal Republic)
1975		
July 6-11	XXV IUPAC Congress (Organizing Committee, XXV IUPAC Congress, POB 16271, Tel Aviv, Israel)	Jerusalem (Israel)
August 25-29	IV International Symposium on Chemistry of Carotenoids other than Vitamin A (Dr. O. ISLER, F. Hoffmann-La Roche & Co. AG, Grenzacherstrasse 124, CH-4002 Basel, Switzerland)	Bern (Switzerland)

September XXVIII IUPAC Conference: closed meeting of IUPAC bodies (Executive Secretary IUPAC, IUPAC Secretariat, Bank Court Chambers, 2-3 Pound Way, Cowley Centre, Oxford OX4 3YF, UK) (Spain)

1976

July 12-16 VI International Congress on Catalysis (Dr. D. A. WHAN, Secretary of Organizing Committee, VI International Congress on Catalysis, c/o Department of Chemistry, University of Edinburgh, West Mains Road, Edinburgh EH9 3JJ, UK) London (UK)

CALENDAR OF NON-IUPAC MEETINGS

1974

March 25-27	International Conference on Plastics in Agriculture and Horticulture (Mr. C. A. BRIGHTON, BP Chemicals International Ltd., UK Plastics Department, Devonshire House, Piccadilly, London W1X 6AY, UK)	Ashford (UK)
March 31-April 5	167 National Meeting of American Chemical Society (Mr. A. T. WINSTEAD, American Chemical Society, 1155 Sixteenth Street NW, Washington, DC 20036, USA)	Los Angeles (USA)
April 1-5	Annual Chemical Congress of Chemical Society and Royal Institute of Chemistry (Dr. J. F. GIBSON, Chemical Society, Burlington House, Piccadilly, London W1V 0BN, UK)	London (UK)
April 18-24	International Conference on Excited States of Biological Molecules (Dr. M. D. LUMB, UMIST, POB 88, Manchester M60 1QD, UK)	Lisbon (Portugal)
April 22-26	Analytica 74: International Salon of Biochemical Analysis and I European Congress of Clinical Chemistry (Dr. R. VOGEL, Nussbaumstrasse 20, D-8000 München 2, German Federal Republic)	Munich (German Federal Republic)
May 3	Van't Hoff Centenary Commemoration (Dr. H. J. C. JACOBS, Gorlaeus Laboratories, University of Leiden, POB 75, Leiden, Netherlands)	Leiden (Netherlands)
May 6-8	International Conference on Industrial Waste Water Treatment and Disposal within EEC (W. J. M. COOK, 'Tree Tops', Stavedown Road, South Wonston, Winchester, Hampshire SO21 3HA, UK)	Amsterdam (Netherlands)
May 16-18	VIII International Working and Discussion Meetings of International Association for Cereal Chemistry (Dr. F. SCHWEITZER, Secretary General ICC, Schmidgasse 3-7, A-2320 Schwechat, Austria)	Vienna (Austria)
May 23-26	General Assembly of German Bunsen Society for Physical Chemistry (German Bunsen Society for Physical Chemistry, Carl-Bosch-Haus, Varrentrappstrasse 40-42, D-6000 Frankfurt 90, German Federal Republic)	Kassel (German Federal Republic)
May 28-31	III Symposium on Ion-Exchange (Hungarian Chemical Society, Anker köz 1, H-1061 Budapest VI, Hungary)	Balatonsfüred (Hungary)
May 29-31	I Canadian Sulfur Symposium (Dr. T. W. SWADDLE, Department of Chemistry, University of Calgary, Calgary, Alberta T2N 1N4, Canada)	Calgary (Canada)
June 2-5	LVII Annual Conference of Chemical Institute of Canada (Chemical Institute of Canada, Room 906, 151 Slater Street, Ottawa, Ontario K1P 5H3, Canada)	Saskatchewan (Canada)

June 17-19	International Symposium on Characterization of Adsorbed Species in Catalytic Reactions (B. E. CONWAY, Department of Chemistry, University of Ottawa, 365 Nicholas Street, Ottawa K1N 6N5, Canada)	Ottawa (Canada)
June 24-27	IV International CODATA Conference (Prof. E. F. WESTRUM, JR., Department of Chemistry, University of Michigan, Ann Arbor, Michigan 48104, USA)	Yerevan (USSR)
July 1-5	VI International Symposium on Organo-Sulfur Chemistry (VI Organic Sulfur Symposium, School of Physical and Molecular Sciences, University College of North Wales, Bangor LL57 2UW, UK)	Bangor (UK)
July 8-13	IV International Conference on Thermal Analysis (Hungarian Chemical Society, POB 240, H-1368 Budapest, Hungary)	Budapest (Hungary)
July 16-19	Centenary Celebrations of Society for Analytical Chemistry (Secretary, Society for Analytical Chemistry, 9-10 Savile Row, London W1X 1AF, UK)	London (UK)
August 29-31	XXV Congress of Hungarian Society for Clinical Pathology (IBUSZ, Organizing Committee for Laboratory Congress, H-7621 Pécs, Pf. 69, Hungary)	Pécs (Hungary)
September 4-6	IV European Conference on Thermophysical Properties of Solids at High Temperatures (Dr. B. PIRIOU, Centre de Recherches sur la Physique des Hautes Températures, CNRS, F-45045 Orléans, France)	Orléans (France)
September 8-14	International Solvent Extraction Conference 1974 (Dr. A. NAYLOR, British Nuclear Fuels Ltd., Windscale and Calder Works, Seascale, Cumberland CA20 1PG, UK)	Lyon (France)
September 11-13	International Symposium on Degradation and Stabilization of Polymers (Prof. G. GEUSKENS, Faculté des Sciences, Campus Plaine, Université Libre de Bruxelles, B-1050 Bruxelles, Belgium)	Brussels (Belgium)
September 16-20	V European Symposium on Fluorine Chemistry (Dr. J. F. GIBSON, Chemical Society, Burlington House, Piccadilly, London W1V 0BN, UK)	Aviemore (UK)
September 22-25	International Symposium on Electro-optical Properties of Macromolecular Solutions (Dr. C. HOUSIER, Laboratoire de Chimie Physique, Université de Liège au Sart-Tilman, B-4000 Liège, Belgium)	Liège (Belgium)
September 22-27	IV International Congress of Food Science and Technology (Secretaría del IV Congreso Internacional de Ciencia y Tecnología de Alimentos, c/o Instituto de Agroquímica y Tecnología de Alimentos, Jaime Roig 11, Valencia-10, Spain)	Madrid (Spain)
September 23-27	IV International Carbon and Graphite Conference (Society of Chemical Industry, 14 Belgrave Square, London SW1X 8PS, UK)	London (UK)
September 30 -October 4	X Symposium International de Chromatographie (Prof. G. EMSCHWILLER, GAMS, 8-10 Rue du Delta, Paris IX, France)	Barcelona (Spain)
October 14-20	Corrosion Week '74: European Federation of Corrosion (Secretariat: Scientific Society of Mechanical Engineers, Kossuth Lajos tér 6-8, Budapest V, Hungary)	Budapest (Hungary)
December 2-6	XIX International Dairy Congress (Congress Secretariat, Vigyan Bhavan Annexe, Maulana Azad Marg, New Delhi 110 011, India)	New Delhi (India)

IUPAC

Macromolecular Chemistry — 8 (Helsinki, 1972)

Edited by K. Saarela

This volume includes the plenary and main lectures presented at the eighth international symposium on macromolecules, which was the first to be held in Finland. The papers cover a wide range of topics: theoretical polymer chemistry, polymerization reactions and new polymers, solid state, solution and bulk properties of polymers, polymer degradation and polysaccharides.

1973 468 pp., illustrated 0 408 70516 7 £18.00 or \$54.00

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XXIV IUPAC CONGRESS
Hamburg: 2—8 September 1973

Selected lectures will be published early in 1974 as IUPAC Additional Publications. Each volume will cover one section of the Congress as follows:

Volume 1. Section 1 — High Polymers	208 pp
Plenary and Section Lectures	\$18.00 (£6.00)
Volume 2. Section 2 — Chemistry of Organic	196 pp
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Volume 4. Section 4 — Compounds of Nonmetals	156 pp
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Volume 5. Section 5 — Applied Electrochemistry	190 pp
Plenary and Section Lectures	\$18.00 (£6.00)
Volume 6. Section 6 — Radiochemistry	174 pp
Plenary and Section Lectures	\$18.00 (£6.00)
Volume 7. Section 7 — Symposium on Information	128 pp
and Communication	\$15.00 (£5.00)
Section Lectures and Contributed	
Papers	

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Volumes for the USA and Canada from:

Crane, Russak & Company, Inc.,
52 Vanderbilt Avenue,
New York, N.Y. 10017, USA.

LIST OF ABBREVIATIONS

ACS	American Chemical Society
ASE	Association for Science Education in UK
ASTM	American Society for Testing and Materials
CAS	Chemical Abstracts Service
CBN	IUPAC-IUB Commission on Biochemical Nomenclature
CEBJ	IUB Commission of Editors of Biochemical Journals
CMN	IUPAC Commission on Macromolecular Nomenclature
CNIC	IUPAC Commission on Nomenclature of Inorganic Chemistry
CNOC	IUPAC Commission on Nomenclature of Organic Chemistry
CNRS	Centre National de la Recherche Scientifique in France
CODATA	ICSU Committee on Data for Science and Technology
CQUCC	IUPAC Commission on Quantities and Units in Clinical Chemistry
CS	Chemical Society in UK
FAO	UN Food and Agriculture Organization
FECS	Federation of European Chemical Societies
FGGE	First GARP Global Experiment
GARP	Global Atmospheric Research Programme
IAEA	International Atomic Energy Agency
ICSU	International Council of Scientific Unions
ICSU AB	ICSU Abstracting Board
IFCC	International Federation of Clinical Chemistry
INN	WHO Recommended International Nonproprietary Names
IOC	Intergovernmental Oceanographic Commission
ISE	International Society of Electrochemistry (formerly CITCE)
IUB	International Union of Biochemistry
IUNS	International Union of Nutritional Sciences
IUPAB	International Union of Pure and Applied Biophysics
RECSAM	Regional Centre for Science and Mathematics in Penang, Malaysia
SAC	Society for Analytical Chemistry in UK
SCOPE	ICSU Scientific Committee on Problems of the Environment
SCOR	ICSU Scientific Committee on Oceanic Research
UN	United Nations
UNESCO	UN Educational, Scientific and Cultural Organization
UNISIST	UNESCO-ICSU Programme on International Science Information System
USAN	United States Approved Names
WHO	UN World Health Organization
WMO	World Meteorological Organization

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**INTERNATIONAL UNION OF PURE
AND APPLIED CHEMISTRY**

**INFORMATION BULLETIN
NUMBER 48**

OCTOBER 1974

IUPAC SECRETARIAT

Bank Court Chambers, 2/3 Pound Way
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International Union of Pure and Applied Chemistry
1974

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

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IUPAC INFORMATION BULLETIN

The Bulletin provides a news medium for the various activities of IUPAC, especially of its 50 or so committees which deal with chemical topics needing regulation, standardization or codification. It carries advance information on forthcoming symposia which are to be sponsored by IUPAC together with reports of such meetings which have recently taken place. Coverage is also given to projects in which IUPAC is collaborating with other international organizations.

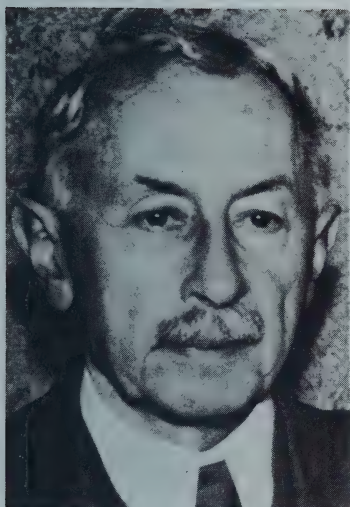
Two series of Appendices to the Bulletin are issued:

- (i) Appendices on Provisional Nomenclature, Symbols, Units, and Standards
- (ii) Technical Reports

In 1974 there will be two issues (Nos. 48 and 49). Annual subscription to the Bulletin, inclusive of the two series of Appendices and postal charges, is US \$9.00 or £3.00 (surface); US \$18.00 or £6.00 (Bulletin and Appendices by air); US \$15.00 or £5.00 (Bulletin by surface and Appendices by air); US \$12.00 or £4.00 (Bulletin by air and Appendices by surface).

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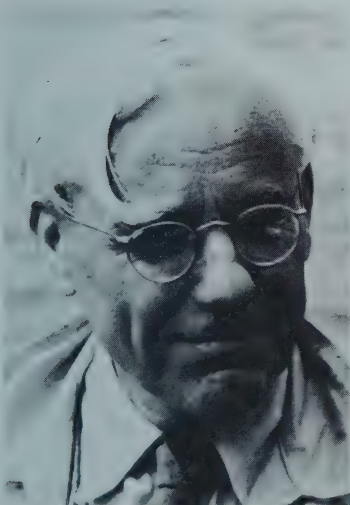
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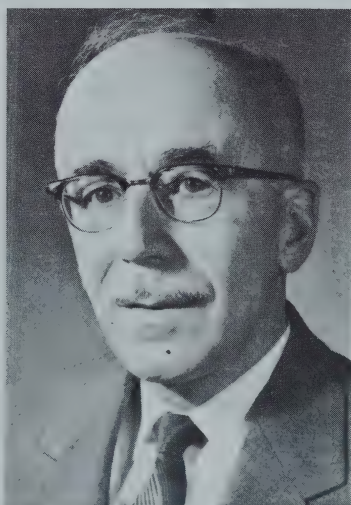
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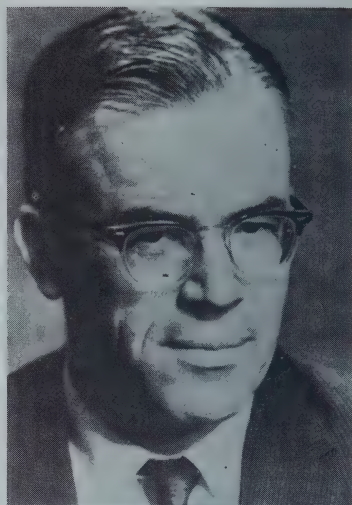
Prof H Erdtman Sweden 1959-1963



Prof L Marion Canada 1963-1965



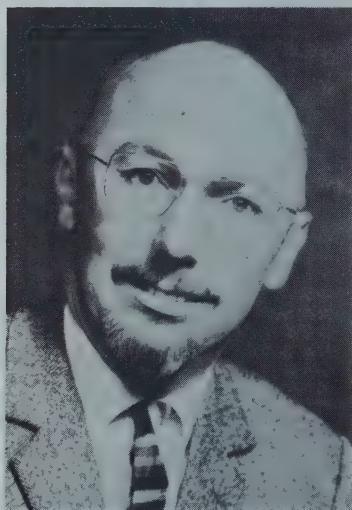
Prof F Weygand Germany 1965-1967



Prof PD Bartlett USA 1967-1969



Prof DHR Barton UK 1969-1971



Prof G Ourisson France 1971-1973



THE PROLIFERATION OF JOURNALS IN CHEMISTRY

Three of our colleagues, namely Profs. C. J. BALLHAUSEN (Copenhagen, Denmark), J. W. LINNETT (Cambridge, UK), and R. Hoffmann (Cornell, USA) have written to me recently expressing their concern at the continued proliferation of commercial journals in chemistry, and asking whether IUPAC can take some appropriate action. They have enclosed a cogent memorandum, signed by eleven distinguished chemists from six countries, engaged in different branches of chemistry, all of them active in research and education and in the affairs of their national chemical societies and being anxious to ensure a proper means of communication in the sciences.

Their memorandum focuses upon the rapid and undesirable increase in number of commercial journals, their frequently high subscription rates, the dilemma of science libraries, and the assumption by publishers that these libraries are 'a captive market'. It suggests that in some cases the standard of refereeing is too low, and that the trend to over-specialization should be deterred on both scientific and financial grounds.

Our colleagues have proposed that libraries should be urged to show more reluctance in buying new commercial journals, and that scientists should refrain from publishing in them. They raise the question whether some international agency could be set up to assess the need for new journals that are proposed, and ask whether IUPAC can take any action of this sort.

This matter has been discussed at recent meetings of the IUPAC Executive Committee and Bureau, whose Members were unanimously in sympathy with the views expressed by our colleagues.

Of course, the difficulty has been recognized by many chemists for some years, and has been considered by committees of national scientific societies among all the complex problems of present scientific publication. In spite of that, it seems to become ever more acute. The fragmentation of science through the mushroom growth of new journals and the trend towards over-specialization is bad for science and the general training of young scientists. The discovery of new physicochemical techniques and their application to chemical problems does not demand the creation of new journals for each of them. Yet this is being allowed to happen at a time when we are supposed to be emphasizing the 'integration' of science, and stressing the importance of inter-relationships. Much of the rush for quick publication by some research workers today is unjustifiable. The introduction of page charges has proved to be not altogether desirable, and is especially damaging when it involves a two-tier mechanism and delay for those who cannot pay. New journals should not be established for their prestige value to either individuals or to nations.

It is probably unrealistic to imagine that any international agency could be set up at present to control the creation of new commercial journals. To a very large extent, however, the power is in the hands of scientists themselves. They need not acquiesce, without serious consideration, to the pressure from publishers whose main interest is financial, nor agree to join Editorial Boards for new journals; and they should restrain themselves and their young colleagues from sending papers to such journals.

Of course, others can help in the wider context. Employers, whether academic or industrial, should attach less importance to the volume of publications of younger scientists, and more to their quality. The slogan 'publish or perish' should be made invalid.

I hope that this statement can be considered urgently by all those connected with the Union, and that they may use their influence towards the desired end.

H. W. THOMPSON
President

28th IUPAC CONFERENCE

Madrid, 2-11 September 1975

The Bureau of IUPAC has decided (Brussels, 31 August-1 September 1974) on the following schedule for the next Conference of IUPAC bodies:

2	September	—	Division Committees, Clinical Chemistry Section
3	} September	—	Standing Committees, Sections, Commissions, Sub-Commissions
4			
5			
6			
7	September	—	Executive Committee, Division Committees, Clinical Chemistry Section
8	September	—	Bureau
9	September	—	Council
10	September	—	Lecture by Lord TODD (UK) <i>Chemistry in a Changing World—A Look Ahead</i>
11	September (am)	—	Council
11	September (pm)	—	New Bureau and Executive Committee

Meetings will take place in the buildings of Consejo Superior de Investigaciones Científicas. Special accommodation arrangements are being made with Hotel Melia Castilla.

Full details will be announced shortly.

REPORTS OF DIVISION PRESIDENTS AND CLINICAL CHEMISTRY SECTION

The following reports of activities since the XXVII IUPAC Conference (Munich, 1973) were presented at the Bureau meeting in Brussels on 31 August-1 September 1974.

PHYSICAL CHEMISTRY DIVISION

Establishment of ad hoc Rules Revision Committee

The Rules of the Physical Chemistry Division were last revised in 1951; subsequent changes in the Statutes and Bylaws of the Union have rendered parts of the Division Rules ambiguous and inoperable. An *ad hoc* Committee has been formed with the Vice-President as Chairman and the President, Secretary, and Prof. D. H. EVERETT as Members. This Committee will submit a draft set of revised Rules to the Division Committee at the 28th IUPAC Conference (Madrid, 1975). It will endeavour to consult closely with the Committee on Statutes and Bylaws to ensure that its proposals remain consistent with any changes that may occur in the Statutes and Bylaws of the Union. It will meet in Paris on 4 September 1974.

Liaison with Commission on Physical Organic Chemistry of Organic Chemistry Division

Following correspondence with Profs. A. KJAER and H. ZOLLINGER, the Physical Chemistry Division Committee has proposed Prof. A. R. H. COLE to provide liaison with the Organic Chemistry Division in matters relating to physical organic chemistry. This is in accord with the report of the *ad hoc* Committee on Physical Organic Chemistry submitted by Prof. ZOLLINGER to the Bureau at the XXVII IUPAC Conference.

Division Newsletter

The Division President, in consultation with the Commission Chairmen, has prepared a Division Newsletter which has been forwarded to the IUPAC Secretariat for circulation to national chemistry news journals with a view to publication. This action was recommended at the Division Committee Meeting at Munich last year.

Environmental Activities

By correspondence with Dr. H. EGAN, the Physical Chemistry Division has offered assistance to the Applied Chemistry Division in the form of technical advice and support on matters relating to environmental activities in those scientific and technical fields in which the Physical Chemistry Division can contribute specialized knowledge.

Activities of the Commissions

All six Commissions of the Physical Chemistry Division have made progress with their programmes which were approved by the Division Committee at the XXVII IUPAC Conference.

Commission I.1 (Physicochemical Symbols, Terminology, and Units). The *Manual of Symbols and Terminology for Physicochemical Quantities and Units* [Pure Appl. Chem. **21**, 1 (1970)] has been updated and the revised

text is now with the printer. Extensive correspondence with the leading theoretical chemists has been generated by the circulation of an informal document 'Expression of Results of Theoretical Chemistry'. This should lead to a more formal report following discussions next year. There has been correspondence with Commission I.5 concerning Mössbauer and other spectroscopic data currently in the Provisional Nomenclature Appendix stage.

Commission I.2 (Thermodynamics and Thermochemistry). A German translation of *Guide to Procedures for Publication of Thermodynamic Data* [Pure Appl. Chem. **29**, 395 (1972)] has been completed. *Experimental Thermodynamics* Volume II has also been set in print and should appear soon. The 1974 *Bulletin of Thermodynamics and Thermochemistry* (No. 17) will be issued in late 1974. Indexes of more recent Bulletins are being set up on computer tape and will be searchable by compound name, etc. (Dr. H. KEHIAIAN). The preparation of a third volume in the series *Experimental Thermodynamics* is under consideration; it would deal mainly with transfer properties under conditions of extreme temperature and pressure. A third volume of *Experimental Thermochemistry* is also under review.

The second and third series from the CODATA Task Group on Key Values for Thermodynamics have been accepted by the Commission; they have been published as CODATA Bulletin No. 10, together with the first series.

The III International Conference on Chemical Thermodynamics was held at Baden bei Wien during 3-7 September 1973. It was organized by Prof. F. KOHLER and augmented by a section on high temperature physicochemical techniques organized by Prof. C. B. ALCOCK. It was the largest international thermodynamics conference yet sponsored by IUPAC. Plans are proceeding for the IV Conference at Montpellier during 26-30 August 1975 under the supervision of Prof. M. LAFFITTE.

A Committee chaired by Dr. J. D. Cox has been established in accord with recommendations made at Munich. It will supplement the coverage on thermodynamic quantities in the IUPAC *Manual of Symbols and Terminology*.

Sub-Commission I.2.1 (Plasma Chemistry) held a Symposium on Plasma Chemistry at Kiel in September 1973, at which IUPAC was represented by the Division President. A similar symposium is being planned for September-October 1975 at Vienna; and also in September 1975 a smaller round table conference on energy transfer between thermal plasmas and condensed phases at Fond Romeu, France. The Sub-Commission is proceeding with its retrospective bibliography.

Sub-Commission I.2.2 (Thermodynamic Tables). There has been extensive activity concerning the IUPAC Thermodynamics Tables Project Centre. The volume on *Ethylenè* was published in April 1974. The draft of the volume on *carbon dioxide* has been circulated for comment; *helium* will soon be ready for circulation and *methane* is in preparation. Financial agreements concerning the continued funding of the project are progressing. Some royalties have been received. Closer liaison with scientists in USSR has followed the visit by Dr. S. ANGUS and he will lecture on the work of the Project at the IV CODATA International Conference at Yerevan in June 1974. In other areas Sub-Commission I.2.2 is considering convening a panel of specialists to study correlating functions for fluid properties and commissioning calculations of ideal-gas thermodynamic properties for wide temperature ranges.

Commission I.3 (Electrochemistry). The recommendation 'Electrochemical Nomenclature' has been completed for final publication in *Pure and Applied Chemistry* [37, 499 (1974)] The Commission will meet in connection with the ISE Meeting at Brighton in September 1974 to discuss planning for activities concerning (a) electrochemistry of nonisothermal systems, (b) inhibition of corrosion and electrocrystallization, (c) electrode kinetics, (d) tables of standard potentials.

Commission I.4 (Physicochemical Measurements and Standards). Revision of the *Catalog of Physicochemical Standard Substances* [*Pure Appl. Chem.* 29, 597 (1972)] is progressing and should be ready for the Madrid Conference. It is also expected that by then new tables will have been prepared of the vapour pressure of water which will take into account the recent work at US National Bureau of Standards. Agreement has been reached with US National Bureau of Standards for publication of the 1961 Ottawa Purity Symposium as one of the NBS Special Publications.

Sub-Commission I.4.1 (Calibration and Test Materials) has been notably active and the following chapters of *Recommendations on Calibration and Test Materials* have been sent for publication in *Pure and Applied Chemistry*, viz. Introduction, Enthalpy, Reflectance, Surface Tension, Optical Rotation. The following chapters are expected to be completed in time for the Madrid Conference: Density, PVT Relations, Thermal Conductivity, Vapour-Liquid Phase Equilibria, Refractive Index, Optical Transmittance and Wavelength, Permittivity, Potentiometric Ion Activities. This programme was reviewed by Prof. H. KIENITZ in a lecture at a Research Symposium on Standard Reference Materials and Meaningful Measurements held at US National Bureau of Standards in November 1973. The Sub-Commission will meet in Gdansk in September 1974 to discuss the furtherance of this programme and other matters.

Commission I.5 (Molecular Structure and Spectroscopy). 'Recommendations for Preservation of Raman Spectra for Cataloging and Documentation in Permanent Data Collections', approved by Council at Munich, was published in *Pure Appl. Chem.* 36, 275 (1973). 'Recommendations for Nomenclature and Spectral Presentation in Chemical Electron Spectroscopy Resulting from Excitation by Photons' will be published (August 1974) in Provisional Nomenclature Appendix No. 37; nomenclature and spectral presentation for *NMR Spectra from Nuclei other than Protons* will appear (August 1974) in No. 38. Provisional Nomenclature Appendix No. 33 (August 1973) dealing with Mössbauer spectra brought several constructive comments from workers in the field and these are now being considered in association with Commission I.1.

Sub-Commission I.5.1 (Infrared and Raman Spectroscopy) is revising and updating Parts I and II of *Tables of Wavenumbers for the Calibration of Infrared Spectrometers* which appeared in 1961. A reprinting is needed and it is proposed that the revised material will be incorporated with Parts III and IV [*Pure Appl. Chem.* 33, 605 (1973)] in a new hard-backed volume covering the complete infrared range (Prof. A. R. H. COLE). Work on 'Definitions and Symbolism of Force Constants' is in progress (Prof. Y. MORINO and Prof. T. SHIMANOCHI) and the leaders in the field are being canvassed with a view to achieving a consensus. Prof. F. A. MILLER will represent IUPAC at the IV International Conference on Raman Spectroscopy at Brunswick, Maine, during September 1974, under IUPAC sponsorship.

Sub-Commission I.5.2 (Storage and Retrieval of Spectroscopic Data) is organizing a session on 'Progress in Handling Spectral Data' at the IV International CODATA Conference at Yerevan in June 1974 (Dr. D. R. LIDE, Jr.). This Sub-Commission is also making a survey to access the needs for recommendations concerning standard formats for spectral data records, compound identification, etc., in chemical spectroscopy and will report on this at the Madrid Conference.

The new *Sub-Commission I.5.3* (Mass Spectroscopy) is formulating a programme to present at Madrid.

Commission I.6 (Colloid and Surface Chemistry). A report on 'Nomenclature for Heterogeneous Catalysis' has been submitted for publication as Provisional Nomenclature Appendix No. 39 (August 1974). A draft version of a report on *Rheological Terminology* has been reviewed by rheologists and a revision is in preparation in collaboration with the International Committee on Rheology (an IUPAC Associate Organization). Work is in progress on a draft report on *Light Scattering* terminology (Prof. J. KRATOCHVIL). Other areas under review are *Dry Electrochemistry* (Prof. R. HAUL) and *Liquid Crystal Phases* (Dr. S. FRIBERG). The report on nomenclature proposals for *Zeolites* is being revised by Prof. R. M. BARRER, taking account of comments made at the Munich Conference and at the 1973 International Conference on Molecular Sieves. Steps are being taken to maintain and develop liaison with ISO/TC 91 (Surface Active Agents) and with the CID definitions of *Flocculation* and *Coagulation* and *Thermodynamic Terminology for Surfaces*. Commission I.6 is cooperating with the CODATA Task Group on Chemical Kinetics in matters concerning *Heterogeneous Catalysis*. The Commission is also working with the Colloid Chemistry Group of the UK Society of Chemical Industry in studies directed to the development of a *Standard Catalyst*.

R. N. JONES
President

11 June 1974

INORGANIC CHEMISTRY DIVISION

The *ad hoc* Committee on Nuclear and Radiochemistry has been set up and approved by the President of IUPAC with the following membership: Prof. S. AMIEL (Israel) Chairman/Convenor, Prof. F. BAUMGÄRTNER (Federal Republic of Germany), Prof. A. C. PAPPAS (Norway), Prof. F. S. ROWLAND (USA), and Prof. L. YAFFE (Canada). This Committee is to report to the Bureau at the 28th IUPAC Conference (Madrid, 1975) on the need to create a Commission on Nuclear and Radiochemistry, interdisciplinary in nature but for administrative purposes to be attached to the Inorganic Chemistry Division.

Commission II.1: Atomic Weights

Council duly adopted the 'Table of Atomic Weights 1973', as proposed by the Atomic Weights Commission and as supported by the Inorganic Chemistry Division of the Union at the Munich Conference in 1973. The preparation of the accompanying full report of the Commission as usual involved appreciable correspondence and consultation between Commission Members. It is considered to be of great importance that new policies and changes in atomic weights are simply and clearly explained to interested chemists throughout

the world. A final manuscript was handed to the publishers in February 1974. Publication in *Pure and Applied Chemistry* is expected in August [37, 589 (1974)].

The Commission has set up an enthusiastic and active body called 'ICAW Mass Spectrometric Evaluation Group'. This Group, composed essentially of five Commission Members and some outside collaborators, is casting a wide net for available data, analyzing their reliabilities and encouraging known experts to attempt new determinations of critically needed isotopic compositions. The Group is attempting to meet this year if funds for such a project can be found.

A draft is now available for the 'Simplified Atomic Weights Table to Four Significant Figures'. The Committee on Teaching of Chemistry wishes to publish this Table.

Commission II.2: Nomenclature of Inorganic Chemistry

The activities of this Commission since the Munich Conference have been concerned largely with preparations for the meeting scheduled for 12-17 August 1974 in UK. In addition to extensive correspondence, Dr. W. H. POWELL and Prof. W. C. FERNELIUS have had two work sessions (one day in November at Columbus and four days in March at Tampa). The following documents have been distributed to Members of the Commission and comments received:

- (i) Nomenclature of Isotopically Modified Compounds (document prepared by Commission III.1)
- (ii) Chemical Nomenclature and Formulation of Compositions of Synthetic and Natural Zeolites (document prepared by Commission I.6)
- (iii) Section D—Nomenclature of Organic Chemistry (document prepared jointly by Commissions II.2 and III.1)
- (iv) Inorganic Polymers (document furnished by a Committee of the Polymer Division of ACS)
- (v) Lanthanoids and Actinoids *vs.* Lanthanides and Actinides (letter from Prof. K. W. BAGNALL)
- (vi) Stereochemical Notation in Coordination Chemistry (document furnished by Dr. POWELL)

In addition, the following documents have been distributed for comment:

- (i) Philosophy and Guidelines (to guide the work of the Commissions)
- (ii) Procedure to Name an Inorganic Compound (a handy guide for the use of the Red Book*)
- (iii) Rules for Naming Isotopically Modified Compounds (rules to be incorporated into the Red Book)
- (iv) Nomenclature of Anions (a document stimulated by a request from Dr. K. CH. BUSCHBECK)
- (v) Systematic Names for Oxo Acids (a study document in an effort to establish how far the Commission may decide to go in substituting systematic for empirical names for oxo acids)

The following documents are in process of being distributed:

- (i) Highly Fluorinated Inorganic Compounds (document revised on the basis of discussions last summer)

Nomenclature of Inorganic Chemistry* [*Pure Appl. Chem.* **28, 1 (1971)]; also available in book form from Butterworths (London)]

- (ii) Nomenclature of Cations (a companion document to the one on anions)
- (iii) Rings and Chains (document revised on the basis of discussions last summer)

Finally, the following documents are in process of preparation:

- (i) Nomenclature of Inorganic Boron Compounds (revision of present rules necessitated by growth of field and criticism from boron chemists)
- (ii) Revision of Table II in the Red Book (an effort to increase the ease of using the rules)
- (iii) Nomenclature of Cluster Compounds (hopefully a final revision of a document under study for 3 years)
- (iv) Locants for Ligands (the complete nomenclature of ligands requires locants in addition to those normally used in organic chemistry. Commission II.2 has asked for help from Commission III.1, but in the meantime is preparing its own document)
- (v) Ligands with Multiple Bonds (a vexing problem which has increased in intensity since the second edition of the Red Book appeared in print)

Commission II.3: High Temperatures and Refractory Materials

The second symposium in the series on Physicochemical Techniques at High Temperatures will be held in 1974 at Toronto. Tentative arrangements are being made for a third symposium at Marseilles in 1975. The object of these meetings is to survey the field of experimental methods for high temperature physicochemical studies, in order to pinpoint certain areas where collaborative studies aimed at setting up standards and standard procedures might be developed.

In the past, some work has been done on vapour pressures of metals which, however, has not been in any way conclusive. By running a number of conferences it is hoped to see more clearly where the present limits of experimental error in such things as the measurement of vapour pressures at high temperatures really lie.

The Commission is considering a cooperative study of electromotive force measurements using the solid electrolyte lime-stabilized zirconia. In order to do this it is necessary to provide samples of the electrolyte which would then be incorporated in cells by a number of workers. A suitable method for the synthesis of this material is under active discussion. A third item is that the first conference on Physicochemical Techniques (Baden bei Wien, September 1973) showed the need for heat capacity standards.

Publication of the *Bibliography of High Temperature Chemistry and Physics of Materials* is continuing satisfactorily. This is made four times a year. The Commission would like to invite some further National Representatives to participate in its work. Finally, the plans for an interim meeting of the Commission in Prague in September of this year are going ahead, although the financial situation of the Division does not allow a full meeting of the Commission, as requested in Munich (1973).

V. GUTMANN
President

2 July 1974

ORGANIC CHEMISTRY DIVISION

Membership

The Division Committee, comprising 9 Members, has welcomed Prof. V. C. BOEKELHEIDE (USA), Prof. S. Itô (Japan), and Prof. J. TOMKO (Czechoslovakia), as new Members, after their approval by the respective National Adhering Organizations.

Budget

The difficult financial situation of IUPAC has been reflected in the activity of the Division of Organic Chemistry. It has been necessary to make moderate reductions in the travel and subsistence expenditures listed in the original budget for Commission III.1 and Section III.4, both meeting in 1974. The Division Committee finds it increasingly difficult to carry the responsibility for useful activity under the prevailing economic conditions.

Commission III.1: Nomenclature of Organic Chemistry

The Commission has maintained its traditionally high and important activity. The main topics discussed at the 1973 meeting in Würzburg will be considered further when the Commission meets at Dorking during 14-19 July 1974:

- (i) Revision of Sections A, B, C, and D of *Nomenclature of Organic Chemistry* (the Blue Book)
- (ii) Finalization of Section E (Fundamental Stereochemistry)
- (iii) Cyclophanes and Polycyclic Arrays of Carbon Atoms
- (iv) Isotopically Modified Compounds
- (v) Natural Products and Their Derivatives (Section F of the Blue Book; also Lipids, Lignins, Prostaglandins, Tetrapyrroles, Carbohydrates, Amino Acids)

The IUPAC-IUB Commission on Biochemical Nomenclature (CBN), which is attached jointly to the Organic Chemistry and Macromolecular Divisions in the case of IUPAC, met at Santiago de Compostela on 3-6 May 1974. 'Nomenclature of Cyclitols' has been published jointly with Commission III.1 [*Pure Appl. Chem.* **37**, 283 (1974)]. Shortly due to appear as Provisional Nomenclature Appendix No. 40 (August 1974) is 'Nomenclature of Corrinoids'.

Commission III.2: Physical Organic Chemistry

This newly formed Commission, comprising 7 Titular Members, has shown considerable enthusiasm and initiative. Those Members attending the II IUPAC Conference on Physical Organic Chemistry in Noordwijkerhout met on 30 April 1974 to consider the far reaching implications of the work of the Commission. It was decided in the first instance:

- (i) to establish contact with other relevant Commissions of the Union
- (ii) to alert the chemical community to the existence of the Commission

With regard to (ii), a report would be published to elicit suggestions from individuals on proposals for standardization of nomenclature in physical organic chemistry.

Commission III.3: Organic Photochemistry

It has been active in compiling information on the best means of reporting experimental data concerning filter transmission and lamp emission. In addition, an informal meeting of the Commission Members attending the V IUPAC Photochemistry Symposium at Enschede (21-26 July 1974) will be held.

Section III.4: Medicinal Chemistry

The Section has continued its worthwhile efforts to achieve worldwide communication within the field of medicinal chemistry. Preparations have been made for the Section meeting at Noordwijkerhout on 8-9 September 1974 in conjunction with the IV International Symposium on Medicinal Chemistry. Final comments are being incorporated by Prof. E. E. SMISSMAN prior to publication of the 'Report on International Education of Medicinal Chemists' as a Technical Report Appendix (No. 13, August 1974) to the *Information Bulletin*. Two drafts report have been circulated by the Chairman (Dr. L. G. HUMBER) of the *ad hoc* Committee on Patent Problems Arising from Structure-Activity Calculations. Prof. A. ALBERT has followed up the question of collaboration of the Section with the Coblenz Society and/or the Sub-Commission on Infrared and Raman Spectroscopy (I.5.1) relative to medically useful substances. He has made similar contact with the Sub-Commission on Solubility Data (V.6.1). In response to a request from IUPHAR, the Section has offered to collaborate in areas of mutual interest.

Symposia

The Division Committee has recommended that sponsorship be given to the following symposia:

V International Conference on Organic Phosphorus Chemistry (Gdansk, Poland: 16-21 September 1974)

International Symposium on Marine Products (Aberdeen, UK: 9-11 September 1975)

VIII International Symposium on Carbohydrate Chemistry (Kyoto, Japan: 16-21 August 1976)

Also, the Division Committee carries the responsibility for initiating and continuing the organization of four periodically recurring series of symposia:

- (i) *Chemistry of Natural Products*. The Division Committee has recommended that sponsorship be given to the X Symposium in the biennial series, to be held in Dunedin during 23-28 August 1976. Negotiations have been opened concerning the meeting place in 1978.
- (ii) *Physical Organic Chemistry*. The Division Committee has recommended that the III Conference in this biennial series be organized in Montpellier in September 1976. Discussions about the location of the 1978 Conference have been started.
- (iii) *Organic Photochemistry*. The VI Symposium in this series, planned for 1976, following the V meeting in Enschede during July 1974, is in a state of preparation.
- (iv) *Organic Synthesis*. Following the I Conference in this series, to be held in Louvain during 26-30 August 1974, the Division Committee is presently involved in attempts to have the II Conference organized in USA in 1976.

Miscellaneous

The Division Officers have assisted Prof. E. CAMPAIGNE in soliciting names of chemists in developing countries, on behalf of the US National Committee for IUPAC, with a view to utilizing chemists and the resources of chemistry in these countries for the benefits of their people.

The Division President cannot withhold his misgivings in connexion with a problem of free admission of two *bona fide* chemists from South Africa to the VII International Symposium on Carbohydrate Chemistry, to be held in Bratislava on 5-9 August 1974, sponsored by IUPAC after recommendation by our Division. It is to be feared that new restrictions in the free admission of *bona fide* chemists to any IUPAC-sponsored meeting will severely threaten the whole future of the Union.

The Division Committee expects to discuss a series of problems of a more general nature at its meeting during the 28th IUPAC Conference (Madrid, 1975).

A. KJAER
President

17 July 1974

MACROMOLECULAR DIVISION

The Macromolecular Division Committee will meet in conjunction with the International Symposium on Macromolecules in Madrid during September. Its Working Party on Structure and Properties of Commercial Polymers has held two meetings: Netherley, 7-8 September 1974; and Brussels, 21-22 February 1974. Also, the Working Party plans to meet at Ludwigshafen on 28-29 November 1974. Its programme on the effect of molecular orientation on the mechanical properties of polystyrene has been completed and a report is being prepared for publication in *Pure and Applied Chemistry*. A report on the PVC rheology programme is being finalized for presentation at the Symposium in Madrid. Amongst the other programmes of the Working Party, that on low density polyethylene rheology is also at an advanced stage with the intention to present a report in Madrid. The Working Party on Molecular Characterization of Commercial Polymers has met twice since the XXVII IUPAC Conference, *viz.* in Paris during November 1973 and in Strasbourg in June 1974. Some successful collaborative results will be presented in a paper at Madrid.

The membership of the newly created Commission on Polymer Characterization and Properties (IV.2) has not yet been settled. Dr. H. WILSKI (Hoechst AG) has been approached to act as the Chairman.

The Commission on Macromolecular Nomenclature (IV.1) met at Santiago de Compostela during 7-10 May 1974. Recommendations on:

List of Standard Abbreviations (Symbols) for Synthetic Polymers and Polymer Materials

Basic Definitions of Terms Relating to Polymers

previously issued as Tentative Nomenclature Appendices to the *Information Bulletin* (Nos. 12 and 13, February 1971), are being finalized for publication in *Pure and Applied Chemistry*. Because of the heavy work load of the Commission Secretary (Dr. L. C. CROSS), Dr. R. B. FOX has been invited to act as Secretary until the 28th IUPAC Conference.

In the series of International Symposia on Macromolecules, coordinated by the Macromolecular Division under the sponsorship of IUPAC, the meeting in 1974 (XXIII) is scheduled for Madrid during 15-20 September. In

1975 the meeting (XXIV) will be in Jerusalem (13-18 July), immediately after the XXV IUPAC Congress. An International Symposium on Macromolecules has also been sponsored by IUPAC at Rio de Janeiro this year (26-31 July), at which the Division President represented the Union. Further meetings in 1974 under the sponsorship of IUPAC are as follows:

XIV Prague Microsymposium on Macromolecules: Crosslinking and Networks (Prague, 26-29 August)

IV Discussion Conference on Macromolecules: Heterogeneities in Polymers (Mariánské Lázně, 2-5 September)

II Aharon Katzir-Katchalsky Conference: Biopolymer Interactions (Amsterdam, 2-6 September)

For 1975, IUPAC has already agreed to sponsor:

IV Bratislava International Conference on Polymers: Modified Polymers, Their Preparation and Properties (Bratislava, 24-27 June)

Symposium on Polymerization of Heterocycles (Ring-Opening) (Lodz-Jablonna, June)

H. BENOÎT
President

12 August 1974

ANALYTICAL CHEMISTRY DIVISION

Owing to budgetary limitations and increasing costs of travel, meetings of Commissions of the Division have had to be severely restricted, generally to those where a time deadline has to be met, *i.e.*, work on nomenclature (Commissions V.3, V.4, and V.5) and on the CEE contract (Commission V.1). In addition, funds were provided to allow a meeting of Sub-Commission V.6.1, in order to get the Solubility Data Project started, and a meeting of the Division Executive Committee. Although no reports have actually been published since the XXVII IUPAC Conference (Munich 1973), there are ten awaiting publication in *Pure and Applied Chemistry* and three reports due to be published as Appendices to the *Information Bulletin*.

Several meetings between Members of the Division Committees of the Analytical and the Applied Chemistry Divisions have taken place in order to strengthen liaison between the two Divisions. Forty-nine ISO Draft International Standards have been distributed for comment by selected Members of the Division. A decision from the Bureau on the extent of collaboration with ISO and on our proposals for IUPAC approval of ISO International Standards is awaited.

It is with the greatest regret that we have to record the death of Dr. A. C. MENZIES (Commission V.4).

Commission V.1: Analytical Reactions and Reagents

The main effort of the Commission continues to be devoted to work on methods of analysis of food additives, in collaboration with Section VI.1 (Food) of the Applied Chemistry Division, in connexion with the IUPAC-CEE Contract. Seven methods being studied for the 1974 programme were discussed at a meeting of the Commission in Paris on 7 May 1974. Other projects under study include colorimetric and fluorimetric methods for analysis of steroids, redox indicators, and complexometric indicators—reports are expected to be finalized in 1975. Further discussions will be held at the next IUPAC Conference on methods for analysis of polyphenols, on

acid-base indicators for nonaqueous titrations, and on primary standards. A report on analysis of amines is nearing completion.

Commission V.2: Microchemical Techniques and Trace Analysis

The change in emphasis of the work of this Commission can be seen from the fact that, of the eleven current projects, eight are concerned with aspects of trace analysis, under two general headings—‘General Aspects of Trace Analytical Methods’ and ‘Trace Analysis Applicable to the Determination of Minor Impurities in Chemicals’. Topics covered in the former include methods of calibration, destruction of organic matter, standard reference materials, analysis of surfaces, and stability of standard solutions; two reports are being processed within the Division. Under the latter heading, topics under study include impurities in oxygen and helium, high purity mineral acids and analytical reagents; one report is in press [*Pure Appl. Chem.* **37**, 481 (1974)], and two more are being reviewed within the Division. Two reports on organic microanalysis have been written and await a decision from the IUPAC Publications Committee on means of publication before final Division approval. Projects still under study are the determination of metals and of carbon, hydrogen, and nitrogen in organometallic compounds, and the analysis of organoboron compounds.

Commission V.3: Analytical Nomenclature

Four reports, approved by Council in 1973, are in press [*Pure Appl. Chem.* **37**, 439, 445, 463, 469 (1974)] and a fifth, recommendations on the usage of the terms ‘Equivalent’ and ‘Normal’, has been submitted for publication as a Provisional Nomenclature Appendix to the *Information Bulletin* (No. 36, August 1974). Projects in an advanced stage include nomenclature of scales of working, the first part (spectrophotometric procedures) of a series on development and publication of methods of analysis, a list of synonyms and trivial names, and nomenclature of ion selective electrodes. Work continues on nomenclature of kinetic methods of analysis, of data processing, and of sampling. The nomenclature of liquid-liquid extraction is being reconsidered to include the requirements of industrial processes. The Commission has been entrusted with the task of compiling a compendium of analytical nomenclature to include all the nomenclature recommendations produced over the years by the Division, updated where necessary.

Commission V.4: Spectrochemical and Other Optical Procedures for Analysis

Work continues on the preparation of reports under the general heading of ‘Nomenclature, Symbols, Units, and Their Usage in Spectrochemical Analysis’. Two reports are nearing completion, one for publication in *Pure and Applied Chemistry* and one for submission to the Division Committee. Projects under active consideration are those on analytical X-ray spectroscopy and associated procedures, for which a draft report is being circulated within the Commission; on systematic classification and description of spectrochemical radiation sources; and on analytical molecular fluorescence spectroscopy.

Commission V.5: Electroanalytical Chemistry

The Commission is continuing its work on solvents and electrolytes; a report on *N*-methylpropionamide is in press [*Pure Appl. Chem.* **37**, 579 (1974)] and another on hexamethylphosphoramide is under review by the Division Committee; a report on purification of electrolytes should be completed in 1975. Compilations of halfwave potentials in dimethylformamide, sulpholane, propylene carbonate, and hexamethylphosphoramide are well under way. A report is in press on scales of ionic activity for standardization of ion-selective electrodes [*Pure Appl. Chem.* **37**, 573 (1974)], and work is in progress on the selectivity of such electrodes, on pretreatment of solid electrodes, and on indicator and reference electrodes in nonaqueous solvents. Studies of conditional diffusion coefficients and of diffusion coefficients in mercury are expected to be completed by the next IUPAC Conference. Tentative reports on the status of the Faraday constant as an analytical standard and on proposed terminology and symbol for the transfer of solutes from one solvent to another have been submitted for publication as Provisional Nomenclature Appendices to the *Information Bulletin* (Nos. 34 and 35, August 1974). The finalized report on classification and nomenclature of electroanalytical techniques and a report on sign convention for currents are to be discussed at a meeting of selected Members of the Commission.

Commission V.6: Equilibrium Data

The first meeting of Sub-Commission V.6.1 (Solubility Data), including representatives of CODATA and Gmelin Institut, has been held at Montreal on 10-12 June 1974. Discussions centred around the needs of other scientific bodies with regard to the collection, evaluation, and presentation of solubility data, guidelines for compilers of data, responsibilities for specific solute-solvent systems, and computerization and publication of data.

Work is proceeding on the gathering of data for the next supplement of 'Stability Constants' by Members of the newly-formed Sub-Commission V.6.2. It is hoped that an IUPAC appeal to trusts and foundations will result in essential financial support for this project.

Two reports on equilibrium constants of liquid-liquid distribution reactions (alkylammonium salt extractants and organophosphorus extractants) are in press (IUPAC Additional Publications: Butterworths, London) and a third (ion exchange equilibrium constants) is in the final stages of Division approval. Two further reports are nearing completion. A series of critical surveys of solution equilibrium constants is progressing well and a draft report on symbols for mixed ligand complexes is being considered by the Commission. Discussions on the development of a data flagging procedure for the retrieval of physical quantities are continuing.

Commission V.7: Analytical Radiochemistry and Nuclear Materials

A report on high energy photon activation is in press [*Pure Appl. Chem.* **37**, 249 (1974)] and one on recommendations for measurement of neutron fluxes is being finalized by the Commission. Work on light elements analysis, nuclear methods for fissile and fertile elements, reference materials for uranium analysis, a critical compilation of radioanalytical data, and on separations in radioanalytical chemistry, is proceeding satisfactorily. Studies on nuclear methods for molecular compounds involved in pollution, on nonnuclear methods for fissile and fertile elements, on charged-particle

induced X-ray fluorescence, and on the state of the art of thorium analysis, have been started. Work continues on examination of reference materials for radiochemical trace analysis; an announcement on three materials was published in *Information Bulletin* No. 46 (October 1973). A report on determination of lead, a key element in environmental pollution, has been submitted to the Division Committee and work on cadmium continues. Problems of nomenclature are being studied and an expanded set of recommendations, including those published as Tentative Nomenclature Appendix 25 of the *Information Bulletin* (June 1972), is being considered within the Commission.

N. TANAKA
President

23 July 1974

APPLIED CHEMISTRY DIVISION

Introduction

The Applied Chemistry Division was established in 1949 and has always had a full and viable programme of work, compatible with the objectives of the Union. The latter objectives can be summarized as working towards the solution of scientific problems of international significance, which are of a pure or applied chemical character and which are not already being studied adequately. Meetings, symposia, research programmes, and financing (directly or otherwise) of any or all of these are among the methods available for contributing to the solution of such problems, the whole being conducted on a nonpolitical basis with the free exchange of scientific opinion between industrial, governmental, and academic interests. The present report relates particularly to the diversification of the Division's programme, with special reference to analytical and environmental aspects.

As at present constituted, the Applied Chemistry Division comprises a Division Committee and six Sections (three of which each have two Commissions), as summarized in the *Appendix*, which indicates briefly the scope of the Division programme for 1973-74. As will be seen, the Sections nominally cover Food, Fermentation, Oils and Fats, Air Quality, Pesticides, and Water Quality. Our views on the structure of the Division in relation to current proposals to revise the IUPAC Statutes (1965) are indicated below.

Applied chemical problems are not the exclusive prerogative of the Applied Chemistry Division, but such problems tend, naturally, to dominate its programme. Equally, the interests of other IUPAC Divisions are not exclusively pure chemistry. But there is need for understanding and exchange of programme information between Divisions. The present report is based on an earlier draft which was given wide circulation within IUPAC, including all Division Presidents and all Chairmen of Sections and Commissions of both the Applied Chemistry and the Analytical Chemistry Divisions. The draft was discussed by the Division Committee at its meeting in Bedford during 11-12 July 1974, when special reports on environmental aspects and on programme diversification, prepared respectively by Dr. S. FREYSCHUSS and Dr. A. F. LANGLYKKE, were also available.

Membership

The basic Membership of the Division comprises the 10 Members of the Division Committee, together with the Titular and Associate Members of the Sections and their Commissions. The total Membership of the Division

is 156 (127 if duplicate Membership is taken into account). The ratio of academic to 'trade and industry' affiliations of the Members is approximately 1:6; that for other Divisions has not been estimated, except in the case of the Analytical Chemistry Division for which the ratio is approximately 2:1. In addition, some 34 National Representatives are accredited to the various Sections and Commissions, mainly Section VI.3. Although IUPAC Company Associates are not individually assigned to specific Divisions, Sections, or Commissions, it is felt that these will often have a special interest in the work of the Applied Chemistry Division. This view is further developed below.

Division Programme

Many, but not all, of the individual programmes of the Division summarized in the Appendix relate to environmental issues and are analytical in character. This is a reflection of the fact that trace analysis is in effect used as an index of safety (or other aspects of environmental quality); that problems arise in the pursuance of greater selectivity and sensitivity in analytical methods to this end; and that environmental issues are themselves matters of continuing national and international importance in both science and politics and in the areas where the two meet. Analytical interests may also be involved when matters of consumer protection are discussed in relation to quality aspects arising from other than direct health considerations, *e.g.*, environmental quality in relation to amenity or the distinction between foods prepared by traditional and by more modern technologies.

For the above reasons, there is already a strong liaison between the Division Committees of the Applied Chemistry and the Analytical Chemistry Divisions. Joint discussions have been held also at Section-Commission levels and both Divisions are anxious to extend these where the Applied Chemistry Division's programme is analytical in character. Steps are, therefore, being taken by both Divisions to extend the liaison in this area.

Whilst, for the reasons already outlined above, it is not wrong that the Applied Chemistry Division should be interested in analytical matters, it is important that its programme should not be devoted to analytical problems to the exclusion of all other problems in the field of applied chemistry. The following general guidelines are proposed for the selection of projects for study:

- (a) Projects should serve common purposes of science and industry; thus, those concerned with standards of measurement, definition, nomenclature, *etc.*, would satisfy this requirement.
- (b) The results should be of general utility: they should be useful to all members of an industry group and may, as well, be useful to governmental agencies, academic institutions, and the general public.
- (c) Projects should not be concerned with features which are competitive with and within industry: they should not be concerned with process development, product identity and quality, product comparisons, except as such studies would be in support of the industry at large or would be designed to protect the consumer or useful to governmental agencies in establishing standards generally designed for protection of the public.

Proposals for new projects should be considered by Sections and Commissions in the light of these guidelines: current programmes should also be considered in a similar way.

The following areas are suggested for the selection of individual problems (projects) for study:

- scientific and technological communication
- resources development (including mineral and biological resources)
- environmental protection
- industrial hazards
- educational needs
- waste recycling (solid wastes management)

Whilst the study of these areas would not be to the exclusion of analytical considerations, projects having a high analytical content should be the subject of closer liaison between the Analytical Chemistry Division and the Applied Chemistry Division.

At the same time, the individual projects from which the Division programme is made up should be the subject of the systematic approval, and where approved, systematic progress review (including where appropriate termination), jointly between the Division Committee and the Sections. This applies both to the new projects and to the current programme. A detailed mechanism for this should be worked out between the Division Committee and the Sections during 1974-75 for implementation in 1975.

Areas of current activity of the Sections should be more specifically defined. In particular, the Section on Air Quality should extend its programme to cover atmospheric chemistry, air quality analysis and chemical aspects of air quality criteria, and pollution abatement; and the Section on Water Quality should cover chemical aspects of limnology, oceanography, hydrology, water quality criteria, and pollution abatement.

At the same time, the pollution abatement aspects referred to immediately above, together with wider aspects of this subject, should (with other environmental issues of interest or potentially of interest to the Division) be studied in depth by the *ad hoc* Committee of three persons formerly envisaged by Council (1971) to discuss and make recommendations for action on the subject of the disposal of solid (and other) wastes. This Committee (the membership of which has not yet been appointed) should thus extend its considerations to wider aspects of the environment, including pollution abatement, the generation, treatment, and disposal of solid wastes, and the possibility of a Section on 'Terrestrial Quality' as a counterpart to Air Quality and Water Quality, which might embrace other pollution aspects at present covered by the Sections on Food and on Pesticides; and the Division Committee recommends accordingly.

The current programme of the Analytical Chemistry Division has been discussed with the President of that Division in relation to the analytical and environmental aspects of the programme of the Applied Chemistry Division. There is little overlap of programmes, but the fuller liaison between the Divisions referred to above should be developed. A special joint meeting will be arranged during the 28th IUPAC Conference (Madrid, 1975) to review the programmes of the two Divisions and to consider further arrangements for continued liaison between them. The Applied Chemistry Division Committee also had the benefit of a note from the President of the Physical Chemistry Division on environmental aspects of his Division's programme. It is felt that a fuller exchange of programme details, in suitably abbreviated form (such perhaps as that used in the *Appendix* to the present report) would be useful between all Divisions.

There is clearly a need to coordinate all aspects of the Division's programme and the Division Committee accepts responsibility for this need. As a longer

term objective it seems reasonable to concentrate, by suitable selection, the present analytical aspects of the Division's programme so as to account for a limited proportion (perhaps half) of the Division's activity; and to diversify further other nonanalytical aspects of the programme.

Other Considerations

The Sections are unusual within IUPAC in that they usually do not form part of the structure of other Divisions, which are made up of Commissions only. The present Statutes are not entirely clear as to the distinction between Sections and Commissions (Sections are apparently to encourage the development of special branches of pure and applied chemistry). These matters have been included in the current proposals for revision put forward by the Committee on Statutes and Bylaws. The proposals relating to the status of Sections were brought specifically to the attention of the Division Committee and were also considered with the diversification issues discussed above, in conjunction with the questions of Titular Membership which were referred to the Division by the Bureau at the latter's meeting in Munich (31 August 1973).

The Division Committee recognizes the need for flexibility of both programme and membership; and it has already commented on the need for systematic review of the former, with the termination of projects where appropriate.

The Division Committee accepts, in principle, the reclassification of the present Sections within the Division as Commissions, with the present Commissions becoming Sub-Commissions (or a series of Sub-Commissions), each based on an individual project, and intends to work towards this objective with effect from September 1975 on the basis that the overall Titular Membership of the Division remains approximately the same in the first instance. To this end it recommends the creation in the first place of eight Commissions, to replace the present six Sections, to be based on:

- Air Quality
- Fermentation
- Food Additives
- Food Contaminants
- Oils and Fats
- Pesticide Residue Analysis
- Terminal Pesticide Residues
- Water Quality

There has not been time to discuss the proposed Commissions with the present Sections of the Division, because the report of the Committee on Statutes and Bylaws only recently became available. Further discussions with the Sections will be necessary during the coming months and the detailed changes in the Division programme will need to be worked out in the 2 years following the 28th IUPAC Conference (Madrid, 1975), in close conjunction with the Chairmen and Members of the Sections (Commissions).

This recommendation also makes for greater flexibility of participation in the work of the Division, through association with individual projects of others in cooperation with Titular and Associate Members as defined by the Statutes and Bylaws. The Division Committee also welcomes the flexibility for change of Membership of (Sections or) Commissions between IUPAC Conferences in appropriate cases.

The programme of the Division is viable and fulfils the criteria indicated under *Introduction*. The views of industry are of special importance and informal discussions between the Division and Company Associates to date confirm this. The Division Committee therefore draws attention to the need to create a mechanism for industry to contribute to (as well as take part in the solution of) the definition of the problems which form the programme of the Division; and to improve the communication between Company Associates and *all* Divisions of the Union in this context. Thus, the Committee gave attention to the organizational diagram (as set out in *Comptes Rendus XXVII Conference—Part A*) and recommends that a new box, 'International Company Associates Group', be inserted between the present boxes 'Company Associates' and 'Bureau', with horizontal linkages to each.

Summary of Conclusions

The views and conclusions of the Division Committee can be summarized as follows:

- (a) The present liaison between the Applied Chemistry Division and the Analytical Chemistry Division should be strengthened and Division programmes should be exchanged on a wider basis.
- (b) Individual projects should become the subject of closer Division review, with fuller definition of objectives and programmes.
- (c) Further attention should be given to bringing the environmental aspects of the programme into closer unity and the *ad hoc* Committee agreed earlier in connexion with solid wastes should now be activated in this wider context.
- (d) An additional area of diversification should be developed in accordance with guidelines proposed.
- (e) Proposals to bring the structure of the Division into line with that of other Divisions by reclassifying the present Sections and Commissions are accepted, in principle, with recommendations for the further discussion and implementation of these over the next 3 years.
- (f) The greater flexibility of participation which (e) above, together with other proposals, implies is also welcomed; and the prospect of a fuller participation by industry and Company Associates.

Subject to their approval by the Bureau, it is proposed to put these recommendations into effect along the lines indicated.

14 July 1974

H. EGAN
President

Appendix—Programme 1973-4

Section VI.1: Food

1. Specifications for purity of food additives (CEE)
2. Specifications for single cell proteins
3. Specifications for dispersal solvents
4. Methods of analysis for tin in food
5. Methods of analysis for zinc in food
6. Rapid methods for assessing food quality
7. Rapid methods for assessing food contamination
8. Rapid methods for assessing food misrepresentation

Commission VI.1.1: Food Additives

1. Detection of nitrosamines in food
2. Detection of polynuclear aromatic hydrocarbons in food
3. Multidetecion methods for antioxidants in food

Commission VI.1.2: Food Contaminants

1. Detection of mercury in foods
2. Detection of lead and cadmium in foods
3. Detection of mycotoxins in foods
4. Methods for specifications for single cell proteins
5. Organization of symposia

Section VI.2: Fermentation

1. Sponsorship and organization of symposia
2. Standards for single cell proteins
3. Education in bioengineering
4. Microbiological aspects of waste-water purification
5. Symbolized terms for quantities and units used in fermentation technology

Section VI.3: Oils and Fats

1. Standard methods for analysis of oils, fats, and soaps
2. Determination of *trans*-fatty acids by differential infrared spectrophotometry
3. Fatty acid derivatives and related products (soap, fatty alcohols, fatty amines, and their derivatives)
4. Glycerine, derivatives and related products (polyglycerols, polyglycerol ester emulsifiers, monoglycerides, etc.)
5. Lecithin and derivatives

Commission VI.3.1: Oils and Fats

1. Melting behaviour of fats
2. Estimation of total oxidized fats
3. Fatty acid composition of butter fat
4. Estimation of tocopherols in oils and fats
5. Estimation of *trans*-fatty acids
6. Pesticide residues in oils and fats

Commission VI.3.2: Soap and Oleochemicals

1. Fatty acid derivatives (soaps, alcohols, amines, amides)
2. Glycerine and derivatives
3. Lecithin and derivatives

Section VI.4: Air Quality

1. Measurement of acidic aerosols and their effect
2. Examination of analytical methods for asbestiform minerals and related inorganic fibrous materials
3. Manual of methods
4. Carbon monoxide in air
5. Development of indicator tubes for hydrogen chloride in air
6. Development of indicator tubes for lead dust in air
7. HDF, tolylene diisocyanate, and vanadium in air
8. Atomic absorption determination of cadmium, lead, and vanadium in air

Section VI.5: Pesticides

1. Liaison with international agencies on problems of pesticide detection and determination
2. Organization of international congresses of pesticide chemistry
3. Policy relating to membership and work of Commissions VI.5.1 and VI.5.2

Commission VI.5.1: Terminal Pesticide Residues

1. Residues of organochlorine and metabolite compounds
2. Hexachlorobenzene residues
3. Residues of organophosphorus compounds and their metabolites
4. Herbicides including metabolites and impurities
5. Residues of carbaryl and other carbamates and their metabolites
6. Nature of residues of fumigants
7. Fungicide residues
8. Residues of other unclassified pesticides

Commission VI.5.2: Pesticide Residue Analysis

1. Liaison with FAO and Codex Committee on Pesticide Residues
2. Determination of residues of organochlorine compounds
3. Determination of residues of organophosphorus compounds
4. Determination of residues of carbamate compounds
5. Determination of residues of fumigant compounds
6. Determination of residues of fungicide compounds
7. Recommendations relating to acceptable methods of pesticide residue analysis

Section VI.6: Water Quality

1. Water pollution abatement in the pulp and paper industry
2. Water pollution abatement in the organic chemical industry
3. Water pollution abatement in the food industry
4. Phenolic waste abatement in water
5. Organization of II International Congress on Industrial Waste Water (Stockholm, 4-6 February 1975)
6. Organization of a section of XXV IUPAC Congress (Jerusalem, 6-11 July 1975)

CLINICAL CHEMISTRY SECTION

A major event was the meeting of the Section Officers at the time of the I International European Congress of Clinical Chemistry (Munich, 21-26 April 1974). Also, all four of the Commissions held meetings. The Members of the new Commission of Toxicology met together for the first time and it became apparent at once that this would be an active and productive group. Several Members of the Section were able to obtain funds from sources other than IUPAC and with this help it was possible for all Members to attend the meetings except Prof. D. H. CURNOW (Australia).

A number of National Representatives were able to attend the Section meeting in Munich and also it was possible to hold a dinner meeting, with funds provided by the Warner-Chilcott Laboratories, a Company Associate

of IUPAC, to which the National Representatives were invited. It is obviously important for these persons to become more familiar with the activities of the Section.

The Section has given its approval for sponsorship of the IX International Congress of Clinical Chemistry (Toronto, 13-18 July 1975). All details have now been worked out and approval has been obtained for IUPAC to sponsor this event, which will attract clinical chemists from around the world. Thus, the close ties between the Section and IFCC are being maintained. This is also signified by the approval given for Dr. D. B. TONKS (Chairman) and Dr. M. ROTH (Secretary) to represent IUPAC on the Executive Board of IFCC. Dr. ROTH attended the January 1974 meeting of this Board. Among the important matters discussed were the reports of the Expert Panels of the Committee on Standards, and the formation of two additional Panels, one concerned with automation and instrumentation, the other with calcium and magnesium.

Dr. ROTH has been establishing contacts with WHO through Dr. R. MORF (official representative of IUPAC to WHO). The Section has signified its willingness to assist WHO in questions concerning education, standardization, and quality control in clinical chemistry. The Members are anxious to make their expertise available to WHO for the improvement of clinical chemistry around the world, and Dr. ROTH has asked Dr. MORF to bring this to the attention of the WHO General Assembly and the Executive Board of WHO.

Dr. R. DYBKAER attended the IUPAC-IUB Commission on Biochemical Nomenclature meeting in Santiago de Compostela in May 1974. Of special interest to clinical chemists was the discussion on quantities and units in enzymology and the problems related to the definition of 'katal' as a unit for *either* enzyme activity *or* for catalytic amount of enzyme. There are supporters for each of these versions and a full discussion of the problem was held at the Commission meeting. This problem was also thoroughly discussed, at the instigation of Dr. ROTH, at the meeting of the Section Officers in Munich this year and it was finally decided not to interfere with publication of the recommendations of the Commission on Quantities and Units in Clinical Chemistry, as edited by Dr. DYBKAER.

One of the major problems of the Section is undoubtedly its status in IUPAC. This problem was discussed at length at the Officer's meeting in Munich and a previous decision to seek Division status was confirmed unanimously. A preliminary brief supporting this proposal, prepared by Dr. TONKS, was read at the meeting. Several changes and additions were suggested and it was then agreed that this proposal should be sent for presentation to the Bureau at its meeting in Brussels during August 1974. It was very definitely the feeling of the Members that the discipline of clinical chemistry was now of sufficient scope and importance to warrant recognition comparable to the other major fields of chemistry. And it was emphasized that only this body represented in IUPAC the area of biochemistry.

Commission on Automation

The Commission has been working on a final version of the document 'Recommendations Concerning the Ideal Attributes of Instruments Intended for Automated Analysis in Clinical Chemistry'. This has now been completed and has been submitted to the Secretariat to obtain approval for publication as a provisional document. It deals with the several analytical

steps from specimen collection and sampling to the calculation of results and reporting. It stresses the requirements for high quality work and is expected to be especially useful to manufacturers designing new automated instruments. A start has been made on two documents concerned with (a) manufacturers description of automated equipment, and (b) evaluation of new automated equipment. Various portions of these documents have been allocated to individual Members of the Commission for writing.

The proposal for IFCC to form an Expert Panel on Instrumentation has been discussed and it has been decided that such a Panel would serve a useful complementary function to the work of the Automation Commission. It is considered that future work of the Commission will inevitably be slanted towards consideration of data processing techniques in clinical chemistry.

Commission on Quantities and Units

A draft on kinds of quantities in absorption spectrometry has been finalized and another on emission spectrometry is being prepared. The Commission reports that SI units are gaining increasing acceptance, with UK entering its second phase of implementation this year and Australia making changes also this year. Serious preparations are under way in Austria, France, German Democratic Republic, Switzerland, and Sweden. The question begins to be contemplated in USA.

The two documents 'Quantities and Units in Clinical Chemistry: Recommendations 1973' and 'List of Quantities in Clinical Chemistry: Recommendation 1973' have been sent in their final form for publication in *Pure and Applied Chemistry* [37, 517 and 547 (1974)] and corrected proofs have been returned.

Several publications on quantities and units in clinical chemistry have appeared in the recent literature and a list of these has been included in the minutes of the Commission meeting held in Munich in April of this year (see pp. 33). Prof. R. HERRMANN is preparing a translation of the article which appeared in *Standard Methods of Clinical Chemistry* (Volume 6, 1970) and the result will be an official version for Austria, Switzerland, and Federal Republic of Germany produced by a Joint Commission under the Chairmanship of Prof. J. BÜTTNER. The kinds of quantities 'Activity' are being considered by Mr. J. C. RIGG of the Commission and it has been decided to contemplate ionic strength, pH, affinity, standard chemical potential, absolute and relative activity, activity coefficients, osmolarity, degree of association, equilibrium constant (c), rate of reaction, pK, and Michaelis constant.

The next scheduled meeting for the Commission is set for the 28th IUPAC Conference (Madrid, 1975). However, because several documents are in preparation it is hoped to meet before then, first at the time of the meeting of the IFCC Committee on Standards (October 1974) and also at the time of the IX International Congress of Clinical Chemistry. IUPAC would not be asked to finance these meetings.

Commission on Teaching

The major effort of this Commission has been the preparation of a monograph on the teaching of clinical chemistry in the world, the role and responsibility of clinical chemists, and the requirements for their education. A penultimate draft was submitted to IUPAC in August 1973, but in January 1974 advice was received from the Committee on Publications that the monograph was too long for publication in its present form. It was suggested

that a shortened version be prepared for publication in the *Information Bulletin* of IUPAC and this is being done. Other avenues for publishing the entire monograph, which has been completely revised, chapter by chapter, are being investigated in cooperation with IFCC. The Commission is in process of collecting from each country the latest available figures on the number of graduate students working in the subject of clinical chemistry and also the existing regulations about education and training.

The Commission is investigating the following topics for future activities:

- Training of senior technologists
- Possible training of speciality technicians
- Audio-visual programmes for use in teaching
- Teaching of clinical chemistry in medical education
- Training in developing countries

The last of these topics is considered to be particularly pressing and potentially fruitful. Two of the Members of the Commission (Profs. M. RUBIN and P. LOUS) have had the opportunity recently of discussing teaching problems and training programmes with colleagues and health authorities in Latin America and South East Asia, respectively.

The Commission wishes to state that an increasing understanding of the role of clinical chemistry in health care systems is being met with all over the world. The problems of standardization, of methods and reagents, of reference materials, and of methods for measuring the quantity and quality of work, are coming up for consideration in many countries and also in international organizations such as WHO.

Commission on Toxicology

This Commission was created at the XXVII IUPAC Conference (Munich, 1973). Prior to that time, Prof. F. W. SUNDERMAN, Jr., proposed Chairman of the Commission, had suggested the names of several persons for Membership. Following acceptance of the Commission, the names of these persons were submitted to the Executive Committee of the Union for approval, and the Commission now has four Titular Members (including Prof. SUNDERMAN) and three Associate Members. A fourth Associate Member has been proposed.

The Commission held its first meeting in Munich on 30 April 1974. As a result of that meeting, the following documents were produced:

- (i) Activity Report
- (ii) Statement of Scope and Terms of Reference
- (iii) Proposal for an International Symposium on the Clinical Chemistry and Chemical Toxicology of Lead (being planned for early 1976. It has been approved by the Clinical Chemistry Section Committee)
- (iv) Recommendations regarding Changes and Additions to the Membership of the Commission
- (v) List of Names and Addresses of Confirmed and Provisional Members of the Commission
- (vi) Budget Proposal

Since the Munich meeting, the Members of the Commission have been occupied with the planning of the 1976 Symposium on Lead. The financing of this event is, of course, of great importance, and IUPAC has been approached for sponsorship and partial funding. It is planned to solicit the remainder of the required funds from other interested bodies and com-

mercial companies interested in the toxicology of lead. Because of the large amount of work which must be done for the Symposium, it is essential to have a meeting of the Commission early in 1975. Plans are being made to hold this meeting in London during January. The Symposium is considered to be especially important not only because it will be the first major effort of the Commission, but also because the topic selected has great current significance.

10 July 1974

D. B. TONKS
Chairman

REPORTS OF IUPAC BODIES

MACROMOLECULAR DIVISION WORKING PARTY ON STRUCTURE AND PROPERTIES OF COMMERCIAL POLYMERS

Brussels, 21-22 February 1974

Present: Dr. A. J. DE VRIES (Chairman), Dr. M. CARREGA (Secretary), Dr. G. AJROLDI, Dr. A. C. BASKETT, Dr. J. CHAUFFOUREAUX, Mr. S. D. EAGLETON, Dr. M. FLEISSNER, Mr. A. GHIJSELS, Dr. J. HEIJBOER, Dr. R. JACOB, Prof. A. S. LODGE, Dr. J. MEISSNER, Dr. H. H. MEYER, Dr. R. N. PITTILO, Dr. A. PLOCHOCKI, Dr. W. RETTING, Dr. A. K. VAN DER VEGT, Mr. J. L. S. WALES, Mr. J. YOUNG, Dr. J. ZELINGER.

Meeting held at Netherley (7-8 September 1973) *

Both Dr. MEISSNER and Mr. WALES confirmed that they would present the reports on LDPE and PVC rheology at the IUPAC International Symposium on Macromolecules in Madrid (15-20 September 1974). Dr. CHAUFFOUREAUX would send within 3 weeks the abstract of the final report on the mechanical properties of PVC. The complete report had been published in *Pure and Applied Chemistry* [35, 315-351 (1973)]. Mr. EAGLETON would contact Dr. JONES to ask him to send to Dr. DE VRIES, as soon as possible, the slightly revised version of his report on the polystyrene programme to be published in *Pure and Applied Chemistry*. Dr. AJROLDI had recalculated some data of Dr. JONES's report, taking account of the difference in T_g between the samples, and proposed to write to Dr. JONES on the subject.

PVC Rheology Programme

Mr. WALES presented his draft report (1974.2.19), taking account of the interim reports issued since the last meeting: BASF, ICI, Hüls, and numerical data from Rhône-Progil. Dr. CHAUFFOUREAUX had specified the processing conditions of the PVC granules: temperature always lower than 170 °C. It was obvious from the discussion that there were some differences of opinion concerning the results obtained at temperatures lower than 180 °C. Dr. CHAUFFOUREAUX gave some more details on the entrance effect of which Mr. WALES would take account in his final report. BASF was asked to supply more information on the entrance corrections made at 175 °C. Dr. MEISSNER suggested to include in the final report also the extrudate swell data of ICI at 170 °C (Table 4 of the last report by COGSWELL). As to the interpretation of the extrudate swell increase with increasing temperature, Prof. LODGE observed that different explanations were possible. He suggested to modify the text (bottom of p. 9 and top of p. 10): "the change in non-Newtonian behaviour with temperature does not preclude the possibility of a transition from particulate to molecular flow, but does not furnish any evidence for that mechanism".

Taking account of the fact that Mr. WALES's report had been distributed at the meeting, participants were requested to read the report thoroughly and to send any comments to Mr. WALES before 1st April in order to enable him to write the final version of the report, which would be presented at the IUPAC

*See *Information Bulletin* No. 47 (March 1974), pp. 9-13.

Symposium on Macromolecules in Madrid. A summary of this report prepared by Mr. WALES during the meeting was approved and would be sent by him to the Symposium Committee for inclusion in the volume of abstracts.

Proposals for a new programme on PVC rheology, based on the conclusions of Mr. WALES's report, would be discussed at the next meeting. TNO was not able to accept the leadership for a new programme on PVC rheology; other members willing to organize a new programme were requested to distribute a written proposal before the next meeting.

LDPE Rheology Programme

The first draft of the final version of Part I was approved for publication after correction of Table 5 (all numbers had to be multiplied by 10). Dr. MEISSNER would send the manuscript with the original drawings to Dr. DE VRIES, who would submit it for publication in *Pure and Applied Chemistry*.

The first draft of the final version of Part II was presented by Dr. MEISSNER, who asked all members to send their comments on this version before 1st April. It was particularly important that all participating members agreed on the final conclusions (red pages of the report). During the discussion at the meeting, several members drew attention to the importance of crystallinity effects in tension and shear and their dependance on melt elasticity. A revised version of the 'red pages', taking account of the comments received, would be issued by Dr. MEISSNER.

A summary prepared by Dr. MEISSNER with the help of Prof. LODGE was approved at the meeting and would be sent by Dr. MEISSNER to the Symposium Committee in Madrid.

Prof. LODGE reported on the work done by GLEISSE in Karlsruhe on fracture phenomena in silicone oil during flow in a cone-and-plate apparatus and its effect on the time dependance of shear and normal stresses. Studies of these effects were in progress at the Rheology Research Center in Madison of which Prof. LODGE gave some preliminary results.

Mechanical Properties of PVC

Dr. CHAUFFOUREAUX presented in detail the conditions of preparation of the samples. Following a remark made by TURNER, it was decided to condition the test pieces at the temperature of measurement (-20 , 0 , 23 , 40 $^{\circ}\text{C}$) for 24 hours and 1 hour only at temperatures higher than 60 $^{\circ}\text{C}$ (80 , 100 , 120 , 140 $^{\circ}\text{C}$). Eight laboratories had sent the list of measurements they intended to perform; the list was completed at the meeting. Dr. AJROLDI reported that Prof. PEZZIN would participate in the programme on tensile tests at low strain rate and on electron microscopy on ruptured test pieces. Technical University Prague would perform tensile tests at low strain rate, dynamic mechanical measurements, and electron microscopy. Rhône-Progil would do microscopy too; Montedison and Solvay would be the only ones to perform impact tests on filled PVC; ICI could do tensile impact tests at different temperatures. Dr. CHAUFFOUREAUX would send the revised programme to the participants. No new participants on the tests already proposed were needed, but new participants proposing other tests would be welcome. Interim reports on the programme were to be sent, if possible, one month before the next meeting.

Structure and Mechanical Properties of Oriented] High Impact Polystyrene

Dr. RETTING announced that the polymerization of sample BASF I was

completed: the polystyrene matrix would be close to PS A of Monsanto (MWD). BASF II was the commercial product 475 K. Six participants were already known. At the meeting TNO declared itself to be willing to join the programme and to send to Dr. RETTING the list of measurements and material needed. Prof. PEZZIN would participate on low speed tensile tests; he would write to Dr. RETTING. The latter would particularly coordinate mechanical measurements and Dr. ZELINGER characterization experiments. Materials would be delivered within 2 months.

Rheology of Block Copolymers

Dr. VAN DER VEGT commented on the preliminary proposal distributed to all members. It was obvious from the general discussion that a more detailed programme was needed, specifying experimental conditions and the techniques to be used for the study of structure changes (electron microscopy of fracture surfaces of quenched samples after shearing and elongation). A survey of technical and scientific data available on Cariflex 1102 would be prepared by Dr. VAN DER VEGT and Mr. GHIJSELS and sent to all participating members, together with a definite programme and information on preparation conditions of test pieces. A stock of material would be set apart by Shell, sufficient to supply all participating members with homogeneous samples. The following members had expressed an intention to participate: BASF, Borg-Warner Chemicals, Hoechst, Hüls, ICI, Prof. LODGE, Montedison, Dr. PLOCHOCKI, Rhône-Progil, TNO. (After the meeting a letter was received from Prof. G. V. VINOGRADOV, who also intended to participate in the programme). Samples would be distributed within 2 months in order to enable the participating members to start preliminary studies.

New Members

New applications for membership had been received from Firestone and Xerox. In a discussion of the usefulness of admitting new members, it was agreed that there was no use in multiplying the same kinds of measurement in too many laboratories, but it would be more worthwhile to apply new techniques of theoretical and experimental investigation. New members would, therefore, be particularly welcome if they proposed to carry out original types of investigation. In any case, all members had to comply with the rules of the Working Party, especially with the first rule (see *Appendix*) which after some discussion and a vote was amended to define more precisely what active membership meant: not only to carry out measurements or theory but also to attend regularly meetings in order to discuss the results obtained in the programmes. It was decided to send to all new applicants the list of rules of the Working Party and the list of the actual and future (if known) programmes with the names of the participating members.

Units

After a vote it was decided to use only SI units in all future reports of the Working Party.

Next Meeting

At the kind invitation of BASF the next meeting would be held in Ludwigshafen on 28-29 November 1974. Prof. LODGE expressed the hope that at future meetings more time would be available for scientific and technical

discussions. The Chairman agreed with Prof. LODGE and promised to take account of this proposal in planning the agenda of future meetings.

M. CARREGA

APPENDIX: Rules for the Working Party

1. Membership is free to all laboratories intending to participate actively in at least one of the programmes. Active participation means: to make measurements and/or theory and to discuss them and to attend regularly the meetings dealing with the programme(s) in which the member is participating.
2. Members who are no longer able to participate actively are invited to resign from membership.
3. Each participating laboratory may delegate one or several members but correspondence will be preferably addressed to one member to be chosen by the laboratory, except by special request from a member laboratory.
4. Interim reports will be sent by the authors to all participating members in the programme concerned, with copies for the Chairman and the Secretary.
5. Progress reports written by the leader of the programme will be sent to all members of the Working Party.
6. Final Reports to be published in *Pure and Applied Chemistry* or any other scientific journal have to be submitted for approval to all members participating in the programme, if possible after a general discussion during a Working Party meeting. An Abstract of each Final Report will be prepared by the author(s) for publication in national and international journals in the field of polymers and plastics. In the Abstract full reference will be given to the published Final Report.
7. A copy of mail concerning the Working Party exchanged between members should be sent to the Secretary by the authors.

COORDINATING COMMITTEE FOR ANALYTICAL METHODS FOR CEE AND IARC (CCAM)

Oxford, 6 April 1974

Present: Prof. R. TRUHAUT (Chairman), Prof. F. PELLERIN (Secretary), Prof. R. BELCHER, Dr. H. EGAN, Dr. R. MARCUSE. In attendance: Dr. M. WILLIAMS and Mr. R. J. M. RATCLIFFE (IUPAC Secretariat).

Minutes of Previous Meeting (Munich, August 1973)

The French text was adopted after several minor modifications had been agreed. The English translation would be published in *Comptes Rendus XXVII Conference* (pp. 83-85). Prof. BELCHER indicated that he was continuing the 'wall chart' and Members of the Committee thought that it would be particularly useful in the establishment of future contracts.

Standing Orders of Executive Committee regarding Coordinating Committee

After an exchange of views on the draft Standing Orders prepared by the Executive Secretary, it was agreed that the Coordinating Committee should be composed of a Chairman, a Secretary, and six other Members. In addition to the five persons present on this occasion, it was thought essential for one of the three remaining places to be filled by Dr. P. L. SCHULLER, Director of the Rijks Instituut voor der Volksgezondheid at Bilthoven. Dr. SCHULLER was highly competent with respect to the analytical methods being studied for fulfilment of the IUPAC-CEE contracts.

Meeting in Brussels: 13 November 1973

Prof. TRUHAUT recalled that in October 1973 the CEE authorities had sought a meeting for establishment of the 1974 contract, emphasizing the urgency for their financial authorities. He was unable to go and delegated Prof. PELLERIN who accompanied the Executive Secretary to Brussels. Dr. WILLIAMS had reported subsequently on the meeting, a copy of his report being sent to each Member of the Coordinating Committee. Unfortunately, the previous efforts of Prof. TRUHAUT to increase the subvention to IUPAC for completion of the contract failed because CEE, fully conscious of the continuing inflationary trends, could not increase its budget. On the other hand, CEE had decreased the number of methods to be submitted under the 1974 contract. It had expressed the wish to see established methods concerning purity criteria specifically for a certain number of additives; the list of methods had been established by CEE.

Methods for 1974 Contract

The Coordinating Committee studied each of the methods sought by CEE.

1. *Fatty Acids in Lactic Acid (E270)*. Dr. EGAN suggested again a method based on the absence of foreign odour. The Coordinating Committee thought that specific research of fatty acids implied the use of gas chromatography. The introduction of such a method could not be achieved without a general method describing the conditions to be used for gas chromatography.
2. *Salicylic Acid in p-Hydroxybenzoic Acid, its n-Propyl Ester, and their Sodium Derivatives (E214 to E217)*. Prof. PELLERIN recalled that this method had been circulated and accepted by Members of the Food Section and Commission V.1, but it had not been sent to CEE in 1972. It would be attached to the methods for the 1974 contract with a fresh circulation.
3. *α -Naphthol in Sodium o-Phenylphenate (E232)*. The method circulated in 1973 (7/73) dealt with α -naphthol in o-phenylphenol. It had been presented by Dr. SCHULLER, who proposed in his comments a method adapted to sodium o-phenylphenate. Prof. PELLERIN would rewrite this method according to the proposals of Dr. SCHULLER and send him the text for his approval.
4. *Sulphur Trioxide in Sulphur Dioxide (E220)*. The method would be established by Prof. BELCHER and Dr. EGAN.
- 5 and 6. *Organic Chlorine in Benzoic Acid and the Benzoates of Sodium, Potassium, and Calcium (E210 to E213)*. The method circulated in

1973 (10/73) related to total chlorine. This was remarked upon during circulation in 1973 and the method was not sent to CEE. Prof. PELLERIN would undertake to present a method for inorganic chlorine, which would be attached to the other method (10/73) for circulation.

7. *Nonvolatile Matter in Sulphur Dioxide (E220)*. The Coordinating Committee discussed the need for such a method. Prof. PELLERIN would obtain the advice of Dr. CHAIGNEAU, Research Director of CNRS in France, a specialist in gas analysis.
8. *Nitrites in Potassium Nitrate (E252)*. This method had been sent to CEE under the 1973 contract (14/73).
9. *Oxalates in Calcium Citrate (E233)*. The method would be adapted from method 28/72 RE.1 by Dr. EGAN.
10. *Reducing Substances in Calcium Lactate (E327)*. Dr. MARCUSE would adapt method 23/69 to the case of calcium lactate.

Thus, with the exception of methods 2 and 8, and of method 7, which was dependent on the advice of a specialist in gas analysis, the other methods would be circulated according to the following timetable:

- Prepared methods to IUPAC Secretariat before 1 May 1974
- Distribution of methods to Food Section and Commission V.1 before 20 May 1974
- Comments to Prof. PELLERIN (Hôpital Général Emile Roux, F-95600 Eaubonne, France) before 20 June 1974
- Circulation of report by Prof. PELLERIN before 1 July 1974
- Final examination of methods by Coordinating Committee on 30 July 1974 at The Hague
- Editorial revision (Dr. A. J. COLLINGS, Dr. M. KAPEL, and Prof. PELLERIN) by 15 September 1974
- Despatch to CEE during October 1974

Discussions then took place on the important question of the final form of methods submitted to CEE under the terms of the contracts. Over and over again the Chairman and Secretary had contacted the CEE authorities to signify the major interest of the Coordinating Committee in receiving suggestions or criticisms from CEE on the methods submitted by IUPAC. In this connexion a meeting had been scheduled for February 1974, but unfortunately CEE did not succeed in holding the meeting. This had resulted in an accumulation of methods for which no comments from CEE had ever been received by IUPAC. Prof. BELCHER remarked appropriately that it would not be possible to study at a single session the comments on a large mass of documents, and it would take a long time to carry out the truly serious work.

Limit Test for Arsenic

Having received a copy of the document sent to CEE in fulfilment of the 1973 contract, Dr. SCHULLER had sent several comments on method 25/72 RE.1 (limit test for arsenic). This method was circulated and had been accepted in 1972. Dr. SCHULLER had not at that time made any remarks. The comments of Dr. SCHULLER would be considered and it was decided to send them for study and comment to the two experts who had been particularly concerned with this method by reason of their work and publications

on this subject, Mr. J. L. MONKMAN and Dr. A. HULANICKI. The latter should address their remarks to Dr. SCHULLER and the question would be studied again at the next meeting of the Coordinating Committee, in which Dr. SCHULLER would participate.

'Round Table' organized by Dr. Marcuse at The Hague

Prof. TRUHAUT reviewed the correspondence exchanged with Dr. MARCUSE concerning the project as a result of the last round table organized in Hamburg at the IUPAC-IUFoST Symposium on Contribution of Chemistry to Food Supplies (see pp. 83) on the subject of purity criteria of food additives. Dr. MARCUSE had originally envisaged holding this meeting at Warsaw on the occasion of the meeting of the Food Section in 1974. After contacting Dr. WILMINK, Chairman of the Food Additives Committee of the Joint FAO-WHO Food Codex Commission, it appeared preferable to hold the round table in The Hague on 29 July 1974. He had asked Prof. TRUHAUT, as Chairman of the Coordinating Committee, to help him organize the round table (Hamburg), which had been very successful and created a lot of interest. Prof. TRUHAUT pressed Dr. MARCUSE to continue with the arrangements for 1974 and asked him to define the programme. After an exchange of very general views, the Chairman proposed several items for the agenda:

- Minutes of the Hamburg meeting and general discussion
- To ask a representative of FAO (Dr. R. K. MALIK) to give an account of the action needed by this organization in this field
- To ask Dr. F. LU, Section Head of Additives of WHO and Secretary of the Joint WHO-FAO Committee, to come himself (or delegate one of his deputies) to outline the part taken by WHO in liaison with FAO concerning studies in this same field
- Talk by Mr. D. F. DODGEN who had been corresponding with Dr. MARCUSE
- Talk by Prof. TRUHAUT on the importance of various problems
- Future perspectives

Dr. MARCUSE was already in contact with Dr. WILMINK.

Codex Alimentarius

The Coordinating Committee took note of the report by Dr. H. GUTHENBERG on the meeting of Codex Alimentarius in Budapest (September 1973). It was thought desirable that Dr. GUTHENBERG should supply information on the criteria placed on the choice of methods and analytical standards.

Atomic Absorption: Lead, Copper, Cadmium, Mercury

Dr. MARCUSE informed the Coordinating Committee that studies were in progress leading to special reports (Drs. GUTHENBERG, K. KOJIMA, COLLINGS). The Chairman remarked that CEE would be very happy to have methods established for the determination of these elements by atomic absorption spectroscopy. It should be pointed out to CEE the difficulties raised in studying these very elaborate methods; the establishment of methods based on the use of atomic absorption required considerably more work than the classical methods so far required by CEE. This should be taken into account in fixing the number of methods required in the next contract.

1975 Contract with CEE

The Members of the Coordinating Committee wished a meeting to be organized with CEE with a view to the drawing up of the programme for the 1975 contract.

Date and Place of Next Meeting

The next meeting was agreed for 30 July 1974 in The Hague.

F. PELLERIN

COMMISSION ON QUANTITIES AND UNITS IN CLINICAL CHEMISTRY (CQUCC)

Munich, 18-20 April 1974

Present: Dr. R. DYBKAER (Chairman), Dr. B. H. ARMBRECHT, Prof. R. HERRMANN, Prof. P. MÉTAIS, Mr. J. C. RIGG (Titular Members); Prof. J. HOMOLKA (Observer).

1. The sessions were to be considered as a joint meeting of CQUCC and the Expert Panel on Quantities and Units (EP on QU) of the IFCC Committee on Standards.

2. The minutes of the previous meeting (Munich, 24-28 August 1974: see *Comptes Rendus XXVII Conference*, pp. 105-108) were approved, subject to slight amendments as suggested by Prof. HERRMANN (1973.9.14) and Dr. M. A. PAUL (1973.11.14).

3(i). Dr. ARMBRECHT had contacted Mr. L. ENSTMENGER (Executive Secretary of AOAC) who had advised that the American FDA group on diagnostic products had requested help from AOAC as regards implementation of the results of collaborative studies in this field. AOAC was interested in IUPAC recommendations to avoid duplication. Further, Dr. ARMBRECHT reported that US Congress Committees had held hearings on metrication legislation, but opposing lobbyists seemed to have succeeded in preventing their passage. Finally, Dr. ARMBRECHT said that pending legislation would provide FDA with sufficient authority to deal with diagnostic devices and that the Section on Clinical Chemistry would have an interest in cooperating.

(ii). Prof. HERRMANN had worked on an amended translation into German of the paper in *Stand. Meth. Clin. Chem.* **6**, 223-244 (1970); the result would be an official version for Austria, Switzerland, and Federal Republic of Germany produced by a Joint Commission under the Chairmanship of Prof. J. BÜTTNER. The text was corrected by Dr. DYBKAER and after further discussion it had been accepted by the three National Associations for publication.

(iii). Prof. MÉTAIS had made contact with a Commission on Spectrometry of the French Standardization Organization (AFNOR), consisting of analysts, producers, and biologists. The French Association of Clinical Biology had created a Commission on Quantities and Units to implement the IUPAC-IFCC Recommendations in France.

(iv). Mr. RIGG reported on his several contacts, *i.e.*, with UNISIST and Association of Scientific Editors.

(v). Prof. HOMOLKA reported that he had produced a paper on quantities and units in the Czechoslovak language. The system had not, however, been

introduced in his country as yet.

4. The following publications on quantities and units in clinical chemistry were noted:

ALLGÉN, *et al.*, *Läkartidningen* **70**, 4405-4407 (1973)

D. N. BARON, *J. Clin. Path.* **26**, 729-730 (1973)

Kommission der Schweizerischen, Österreichischen und Deutschen Gesellschaft für Klinische Chemie, *Z. Klin. Chem.* **12**, 180-192 (1974)

R. DYBKAER and K. JØRGENSEN, *Amer. J. Clin. Path.* **61**, 306-307 (1974)

J. HOMOLKA, *Cas. Léč. čes.* **112**, 526-530 (1973)

P. MÉTAIS, *Méd. Prat.* 1974, 45-46

D. S. YOUNG, *New Engl. J. Med.* **290**, 368-373 (1974)

5. The corrected manuscripts of the two Recommendations 1973 (Quantities and Units in Clinical Chemistry; List of Quantities in Clinical Chemistry) had been sent by Dr. DYBKAER to the IUPAC Secretariat for publication in *Pure and Applied Chemistry*. He had just received notice that the first proofs had arrived in Copenhagen and promised to send copies of the corrected proofs to the Members for scrutiny.

6. A second draft recommendation on quantities and units in emission spectrometry was presented by Prof. HERRMANN and discussed together with the second draft recommendation on quantities and units in absorption spectrometry, which had been circulated by Prof. MÉTAIS just before the meeting. It was decided to redistribute and to a certain extent to rephrase the material according to the following provisional scheme:

Part 1. Kinds of quantities for optical spectroscopy in clinical chemistry—General considerations. Consisting of parts of Prof. HERRMANN's draft (1974.4.14) and parts of Prof. MÉTAIS' draft as revised at the meeting (1974.4.18). The latter should be sent by Mr. RIGG to Prof. HERRMANN, who would produce a new draft and send it to Dr. ARMBRECHT for minor corrections. Dr. ARMBRECHT would circulate it before 1974.8.5.

Part 2. Kinds of quantities for description of optical spectrometers. The draft by Prof. HERRMANN would be sent to Mr. RIGG for minor revisions, then circulated. Deadline as for Part 1.

Part 3. Kinds of quantities for molecular absorption spectrometry in clinical chemistry to be constructed by Profs. HERRMANN and MÉTAIS from their present drafts and sent to Dr. DYBKAER. Deadline as for Part 1.

Part 4. Kinds of quantities for molecular and atomic emission spectrometry. The draft would have to wait some time.

7. The kinds of quantities 'activity', *etc.*, had been considered by Mr. RIGG and found difficult to choose and define. It was decided that he would contemplate ionic strength, pH, affinity, standard chemical potential, absolute and relative activity, activity coefficients, osmolarity, degree of association, equilibrium constant (*c*), rate of reaction, *pK*, Michaelis constant.

8. A second draft on transport of components with time (1974.4.1) had been circulated by Dr. DYBKAER. The discussion was cut short due to lack of time. Comments were to be sent to Dr. DYBKAER before 1974.6.30.

9. It was decided to ask the Clinical Chemistry Section for permission to change the following term in Recommendations 1973: 'mean catalytic rate' to 'mean catalytic amount rate' in order to avoid mistaking the former kind of quantity for 'rate of reaction'. [This permission was given by CCS on 1974.4.21.]

10(i). The next meeting of CQUCC (and EP on QU) was scheduled for the 28th IUPAC Conference (Madrid, 1975). In view of the several documents now in preparation it was decided that this meeting was too late. Therefore, the IFCC Committee on Standards should be asked to finance an EP on QU (and CQUCC) meeting during 24-26 September 1974. To save money Prof. HERRMANN graciously offered to arrange the meeting in Giessen. At this meeting Parts 1 and possibly 2 of Item 6 could be discussed together with Item 8. An extra meeting in the Spring of 1975 might be necessary to finalize manuscripts for the provisional recommendation stage.

(ii). The meeting of EP on QU at the IX International Congress of Clinical Chemistry in Toronto (July 1975) would not be financed by IUPAC. Yet, a meeting with EP Associate Members and with other EPs would be valuable. It could be envisaged that attendance in other capacities would make it possible for ARMBRECHT, DYBKAER, and MÉTAIS to attend such meetings if IFCC would pay subsistence allowances only.

11. A letter (1974.1.26) about the IUPAC Solubility Data Project was read out. Dr. DYBKAER would inform Prof. A. S. KERTES that clinical chemical data might be available and important to include.

12. It should be clarified whether IUPAC would demand dissolution of CQUCC in 1977, after existence for 10 years, or if the nature of its subject and the several areas still to be explored would warrant extension of the Commission's life. In the former case, no new Members should be added, but Dr. ARMBRECHT and Prof. MÉTAIS would be suggested for Associate Membership from 1975. In the latter case, a new Member should be nominated at the same time.

13. A letter from Dr. M. ROTH (1974.4.16) to the IFCC Secretary, Prof. J. FREI, advocating the change of IFCC Recommendations 1973 as regards kinds of quantities for enzymes (catalytic amount \rightarrow catalytic activity, and katal \rightarrow mol/s) was discussed with him. The letter restated Dr. ROTH's position already put before the Commission (1972.1.24). The Commission unanimously decided to stand by its text, especially as both views were presented, even if one (catalytic amount and katal) was preferred.

14. Mr. RIGG would circulate for comment an 80-page International Biological Programme publication.

R. DYBKAER

COMMISSION ON AUTOMATION IN CLINICAL CHEMISTRY (CACC)

Munich, 19-20 April 1974

Present: Prof. T. P. WHITEHEAD (Chairman), Prof. H. BÜTTNER, Prof. M. HJELM, Dr. D. S. YOUNG (Titular Members); Dr. J. BIERENS DE HAAN (Associate Member).

1. The minutes of the previous meeting (Munich, 21-22 August 1973) had been published in *Comptes Rendus XXVII Conference* (pp. 103-104).

2. The first day was spent on finalizing the document 'Recommendations Concerning the Ideal Attributes of Instruments Intended for Automated Analysis in Clinical Chemistry'. It was hoped that this document would be dispatched to the Bureau in June 1974.

3. A start was made on two documents concerned with (a) manufacturers description of automated equipment, and (b) evaluation of new automated equipment. Various portions of these documents were allocated to individual Members of the Commission for writing.
4. The proposal for IFCC to form an Expert Panel on Instrumentation was discussed by the Commission. It was decided that such a Panel would serve a useful complementary function to the work of CACC.
5. Future work of the Commission would inevitably be slanted towards consideration of data processing techniques in clinical chemistry.

T. P. WHITEHEAD

COMMISSION ON TEACHING IN CLINICAL CHEMISTRY (CTeCC)

Munich, 19-21 April 1974

Present: Prof. M. RUBIN (Chairman), Prof. P. LOUS (Secretary), Prof. A. L. LATNER, Dr. M. ROTH (Titular Members); Prof. A. DEFALQUE, Dr. C. J. PORTER (Associate Members).

1. The minutes of the meeting held in Munich on 24-26 August 1973 (see *Comptes Rendus XXVII Conference*, p. 109) were approved.
2. The situation regarding publication of the results from the work of the Commission was discussed. The IUPAC Committee on Publications had decided not to publish the whole monograph on teaching of clinical chemistry, but a short summary was wanted for publication in the *Information Bulletin*. CTeCC and IFCC were free to investigate other possibilities and decide upon publication of the whole material through other channels.
3. The essential chapters of the monograph were revised, chapter by chapter, and agreement was reached for content as well as form.
4. The national reports were discussed, especially a condensed version in schematic form. It was decided to collect, if possible with the help of the IFCC Secretariat, for each country the newest available figures for the number of graduates working in the subject of clinical chemistry and the existing regulations about education and training.
5. For the chapter on the history of clinical chemistry, the Commission had in hand one draft written by Prof. LATNER, a table (3 pages) of 'marking events' prepared by Dr. ROTH, and a short draft written by Prof. H. BÜTTNER. Prof. LATNER was willing to rewrite this chapter during the next 2 months.
6. Prof. RUBIN would investigate problems related to the publication of the full report from the Commission.
7. Future activities of the Commission were discussed. Among the items deemed pressing and also potentially fruitful were: training programmes and courses for developing countries (e.g., quality control, instruments); audio-visual aids in the teaching of clinical chemistry; education and training of technologists for special new techniques.
8. A meeting before the 28th IUPAC Conference in Madrid (1975) would be of great importance for the work of the Commission. Prof. RUBIN would investigate the financial possibilities.

P. LOUS

COMMISSION ON TOXICOLOGY IN CLINICAL CHEMISTRY (CToCC)

Munich, 19-20 April 1974

Present: Prof. F. W. SUNDERMAN, Jr. (Chairman), Prof. R. BOURDON, Dr. S. S. BROWN (Titular Members); Prof. M. J. G. MERCIER, Dr. D. B. TONKS (Associate Members); Dr. J. BURET, Dr. H. E. SPIEGEL (Observers).

1. A statement was drafted on the Background, Scope, and Terms of Reference of CToCC. This document was later formally approved by the Section on Clinical Chemistry (74.4.21).

2. Priorities were considered for the programmes of the Commission. Based on these deliberations, first priority was assigned to the organization of an International Symposium on Clinical Chemistry and Chemical Toxicology of Lead, to be held in France during Summer or Autumn of 1976. Concurrent with planning for the Symposium, an interlaboratory survey of the proficiency of lead analyses in blood would be undertaken by Dr. TONKS in collaboration with other Members of the Commission. The second priority was assigned to the organization of an International Symposium on Gas Chromatography/Mass Spectrometry in Clinical Chemistry and Chemical Toxicology, to be organized during 1978. These priorities were later approved by the Section on Clinical Chemistry (74.4.21).

3. Responsibilities were established for organization of the International Symposium on Lead, as follows:—

Financial: Dr. TONKS

Publication: Dr. BROWN

Meeting Arrangements: Prof. BOURDON

Scientific Programme: Prof. SUNDERMAN

Exhibits and Demonstrations: Dr. SPIEGEL

Publicity: Prof. MERCIER

4. The basic organization of the scientific programme for the International Symposium on Lead was developed, and the Chairmen of the scientific sessions were established as follows:—

Metabolism and Molecular Toxicology: Prof. MERCIER

Methods of Lead Analysis: Prof. BOURDON

Measurements of Lead in Specific Body Fluids, Tissues, and Excreta:
Dr. SAVORY

Measurements of Enzymes, Porphyrins, and Porphyrin Precursors:
Drs. BROWN and SPIEGEL

Reference Materials and Quality Control Procedures for Lead
Analyses and Related Tests: Dr. TONKS

Clinical Interpretations, Reference Intervals, and Critical Values of
Laboratory Tests for Diagnosis and Treatment of Lead Poisoning:
Prof. SUNDERMAN

5. A tentative schedule of activities of the Commission was proposed. CToCC planned to meet for 2 days in UK early in 1975 to make decisions regarding the site, dates, organization, financial arrangements, and possible speakers for the International Symposium on Lead. Invitations would be issued to invited lecturers, so that a detailed programme could be formulated at the Commission meeting in Spain during the 28th IUPAC Conference (1975). The programme would be submitted for approval by the Section on Clinical Chemistry and Council during the 28th IUPAC Conference. The

Commission planned to meet for 2 days in France approximately 4-5 months prior to the Symposium, in order (a) to review the abstracts of contributed papers, (b) to inspect the meeting halls, conference rooms, exhibit areas, hotel accommodation, projection and translation facilities, *etc.*, and (c) to review the arrangements for printing of the programmes and publication of the proceedings.

F. W. SUNDERMAN, Jr.

SECTION ON CLINICAL CHEMISTRY (CCS)

Munich, 21 April 1974

A meeting of the Officers of the Clinical Chemistry Section was held in conjunction with the European Congress of Clinical Chemistry (22-26 April), in which Members of the Section Committee and the four Commissions attached to the Section who were in Munich were invited to participate.

Present: Dr. D. B. TONKS (Chairman), Prof. P. LOUS (Vice-Chairman), Dr. M. ROTH (Secretary), Dr. R. DYBKAER, Prof. F. W. SUNDERMAN, Jr., Prof. T. P. WHITEHEAD (Titular Members); Prof. H. BÜTTNER, Prof. A. DEFALQUE, Prof. J. FREI, Prof. J. HOMOLKA, Prof. M. RUBIN (Associate Members); Prof. A. DE LEENHEER, Prof. E. KAISER, Dr. F. L. MITCHELL (National Representatives)—Section Committee; Prof. M. HJELM, Dr. J. BIERENS DE HAAN (Commission on Automation); Dr. B. H. ARMBRECHT (Commission on Quantities and Units); Dr. S. S. BROWN, Prof. M. J. G. MERCIER (Commission on Toxicology); Dr. G. N. BOWERS, Jr., Dr. J. BURET, Dr. A. H. HOLTZ, Prof. D. STAMM (Observers).

Minutes of Section Meeting (Munich, 27 August 1973)

The minutes (see *Comptes Rendus XXVII Conference*, pp. 98-102) were approved, subject to the following changes:

- (i) "A pending problem was to find a name for kinds of quantities where concentrations are expressed relative to the mass of the system" (see p. 99).
- (ii) "There had been much trouble with enzyme units, because biochemists (and IUB) insisted on having a derived unit (katal) to express 'enzyme activity', and would also like to derive a concentration from it (activity divided by volume). This led to problems with dimensions as confirmed by the physicochemists. Despite these objections, an unsatisfactory version of recommendations on Quantities and Units in Enzymology had now been approved by IUPAC-IUB. It had been suggested that the Commission made its own proposal. Of course, even if katal was used as a unit for either enzyme activity or catalytic amount of enzyme, the numerical values would be the same" (see p. 99).

The following matters arising from the minutes were considered further:

- (i) A suggestion from Prof. SUNDERMAN that the Bureau should be asked to consider the motion (see p. 100) for IUPAC to publish a comprehensive glossary of recommended scientific terms, abbreviations, and symbols, was approved.
- (ii) It was hoped that a better structure and functioning of the Interdivisional Committee on Nomenclature and Symbols would soon be implemented (see p. 101).

IX International Congress of Clinical Chemistry (Toronto, 1975)

IUPAC had been offered publication rights for one of the symposia to be held at the Congress. As soon as the main lecturers were known for this symposium, sponsorship of the Union was expected to be granted.

Commission on Automation

Prof. WHITEHEAD presented the work of the Commission. The latter had now prepared a document entitled 'Recommendations Concerning the Ideal Attributes of Instruments Intended for Automated Analysis in Clinical Chemistry'. The final version, which would be ready in a few weeks, would be proposed to IUPAC for publication as a provisional document. It dealt with the several analytical steps from specimen collection and sampling to the calculation of results and report. It stressed the requirements for high quality work and was expected to be especially useful to manufacturers designing new automatic instruments. A second document which was in preparation concerned methods of evaluation of automatic instruments and the information which should be supplied by manufacturers on the performance of their machines.

A joint meeting with the Committee on Standards of IFCC had been held; the creation of an IFCC Expert Panel on Instrumentation appeared very desirable and was expected to occur in the near future. It would work in close cooperation with the IUPAC Commission on Automation which, however, would limit its main tasks to automation and data processing. As a consequence, the motion voted in Munich (73.8.27). "It is proposed that a Commission on Clinical Chemistry Instrumentation be formed as soon as possible" was cancelled.

Commission on Quantities and Units

Dr. DYBKAER presented the work of the Commission. A draft on kinds of quantities in absorption spectrometry had been finalized, and another one on emission spectrometry was in preparation. SI units were gaining increasing acceptance. UK entered its second phase of implementation this year and Australia would change also in 1974. Serious preparations were under way in Austria, France, Federal Republic of Germany, Switzerland, and Sweden. The question began to be contemplated in USA.

The two documents 'Quantities and Units in Clinical Chemistry: Recommendations 1973' and 'List of Quantities in Clinical Chemistry: Recommendation 1973' had been sent for publication in *Pure and Applied Chemistry* and were now at the proof stage. If publication was made jointly by IUPAC and IFCC, approval by the IFCC Council was necessary and this had yet to be given. Recently, criticism had been expressed against the definition of the enzyme unit 'katal'. Dr. ROTH, in his capacity as IFCC Editorial Board member, had written a letter to Prof. FREI indicating that the proposed definition mixed quantity of catalyst and catalytic activity, and expressing his concern about the ambiguity of the term 'catalytic amount'; in his opinion, proposing the 'katal' as a new basic unit was unwise because such a unit, being subject to variations in function of pH, temperature, substrate, activators, inhibitors, etc., did not have the constancy characteristic of the seven accepted basic SI units. Some participants found that Dr. ROTH's remarks

were very late, because the Recommendation had already been accepted by the IUPAC Section in August 1973. Dr. ROTH replied that this acceptance had not been made on the basis of a written text because this was unavailable, but in confidence that the tentative document had been modified in respect of the remarks sent to the Commission.

Dr. BOWERS mentioned that the IFCC Expert Panel on Enzymes also disagreed with the proposed definition of the enzyme unit. The Panel recently issued a tentative document in which the term 'catalytic activity' and the derived unit (mol/s) were recommended for expressing the results of enzymatic analyses. On the other hand, the Committee on Standards of IFCC had accepted the 1973 Recommendations.

The possibility of editing the IUPAC document in its present form with a footnote mentioning the objections raised against the basic unit 'katal' and the term 'catalytic amount' was considered, but it was felt that this would considerably weaken the persuasive strength of a recommendation. After further discussion in which Dr. DYBKAER confirmed his point of view and some participants expressed their understanding of Dr. ROTH's objections, it was decided to proceed with the publication of the two recommendations as edited by Dr. DYBKAER.

Dr. DYBKAER would participate as an Observer at a meeting of the IUPAC-IUB Commission on Biochemical Nomenclature (CBN) to be held in Santiago de Compostela on 7-10 May 1974. He would send a report to the Section Committee.

Commission on Teaching

Prof. RUBIN presented the work of the Commission, which had been devoted to the preparation of a monograph on the teaching of clinical chemistry in the world, the role and responsibility of clinical chemists, and the requirements for their education. The penultimate draft was submitted to IUPAC in August 1973. In January 1974 the IUPAC Committee on Publications advised that the text was of such length that it would have to be shortened considerably if IUPAC was to publish it. It was suggested to publish in the *Information Bulletin* only that part of the manuscript describing the role of the clinical chemist and the appropriate education to be recommended. The April 1974 meeting of the Commission was mainly devoted to the preparation of such a shortened version, which would be ready for submission to the next IUPAC Bureau meeting.

Concerning the future activities of the Commission, certain topics had been proposed which would be given special consideration. These were:

- Training of senior technologists
- Possible training of speciality technicians
- Audio-visual programmes for use in teaching (the Commission could serve as a central international depository)
- Teaching of clinical chemistry in medical education
- Training in developing countries

Prof. WHITEHEAD stressed the importance of teaching in clinical chemistry. Quality control programmes and good instruments were no substitutes for good education, because an understanding of the principles of analyses was essential to the production of good quality results.

Commission on Toxicology

Prof. SUNDERMAN reported on the work of the new Commission, which had met for the first time in Munich. A statement was drafted on the background, scope, and terms of reference of the Commission on Toxicology. After discussion, it was decided to delete a few items from the scope, but otherwise to accept the statement.

As one of its first activities, the Commission planned to organize an International Symposium on Clinical Chemistry and Chemical Toxicology of Lead for 1976. A keynote lecture on the distribution of lead in the biosphere and its implications for man would be followed by several sessions, one of the topics being the analysis of lead in biological materials. Prof. WHITEHEAD thought that the present quality of lead analyses was not satisfactory and he would like good methods to be developed before the Symposium was held. Prof. SUNDERMAN replied that one of the tasks of the Symposium would be to compare critically the different methods of lead analysis. Prof. LOUS suggested that ILO would be interested in the subject and could perhaps be of help in organization of the Symposium.

Proposal to Change Section on Clinical Chemistry to Divisional Status

If this proposal was to be passed to the IUPAC Bureau, it should be supported by strong arguments. Dr. TONKS had therefore prepared a text which he read out and which was unanimously accepted in principle. Dr. BOWERS suggested to include some mention of the economic importance of clinical chemistry instrumentation. According to Prof. BÜTTNER, 20% of the market of analytical instruments was contributed by clinical chemistry. Prof. LOUS would like to have a more complete account on education in clinical chemistry, and to underline in which respect clinical chemistry was a specific discipline. Dr. TONKS agreed to revise the text accordingly and send it to the Titular Members of the Section for approval.

M. ROTH

COMMISSION ON PHYSICAL ORGANIC CHEMISTRY (III.2)

Noordwijkerhout, 30 April 1974

Present: Prof. H. ZOLLINGER (Chairman), Dr. J. R. PENTON (Secretary), Prof. J. F. BUNNETT, Prof. V. GOLD (Titular Members).

Introductory Remarks

Although no meeting of the Commission was scheduled for 2 years after its formation at the XXVII IUPAC Conference (Munich, 1973), the occasion of the II IUPAC Conference on Physical Organic Chemistry held at Noordwijkerhout (Netherlands) from 29 April-2 May 1974 provided an opportunity for those Titular Members of the Commission who attended the Conference to discuss the general purposes and aims of the Commission.

Purposes and Working Methods

It was unanimously decided that the Commission could:

- (i) work by correspondence for the next 18 months;

- (ii) serve a real purpose in setting up a system for the naming of organic reactions, in seeking to develop a rational system for symbolization of the mechanisms of organic reactions, and in clarifying the situation with regard to the definitions used in this field.

Further, it was resolved that in future the Commission should:

- (iii) cooperate with the corresponding Commissions of other IUPAC Divisions;
- (iv) inform the chemical community as a whole that this Commission existed and alert it to the tasks which the Commission would undertake.

Contacts with Other IUPAC Divisions

It was noted with satisfaction that Dr. R. N. JONES, President of the Physical Chemistry Division of IUPAC, had assured the Commission of his full assistance in establishment of a working relationship with the Physical Chemistry Division. The appointment of an Associate Member, Prof. A. R. H. COLE (Australia), for the liaison work between this Commission and the Physical Chemistry Division was in hand.

It was decided that the Commission should establish contact with the other IUPAC Divisions with a view to:

- (i) informing these Divisions of the work of the present Commission;
- (ii) ensuring that the present Commission was fully informed of the work and decisions of the corresponding Commissions within these Divisions;
- (iii) agreeing on an arrangement whereby the communication of these decisions could be easily accomplished, e.g., the appointment of a liaison officer.

Priorities in Tasks

It was decided that the first task of the Commission was to advertise its existence to the chemical community, describing the purposes and aims of the Commission and stressing that suggestions from individuals were welcome. It was emphasized that the adoption of such an approach would greatly facilitate the work of the Commission and would provide information and ideas which would enable the Commission to reach decisions acceptable to the majority of workers in the field. Also, it was emphasized that the very nature of the tasks undertaken by the Commission would certainly arouse interest from organizations which dealt with the compilation and retrieval of chemical data.

With this in mind, two methods of approach were decided upon:

- (i) An announcement of the purposes and aims of the Commission in periodicals and journals such as *Chemical and Engineering News*, *Chemistry in Britain*, *Angewandte Chemie* and, if possible, *Chemical Abstracts*.
- (ii) The preparation of two reports for publication in periodicals and journals.

With regard to (ii), it was suggested that a fairly long report be prepared (ca. 20 typewritten pages) which described in detail the suggestions of the Commission for the naming of reactions, the mechanisms of reactions, and the definitions used in physical organic chemistry. A preliminary draft of the paper would be prepared by the Chairman and Secretary and sent to Members for additions and comments. The second report would consist

of a paraphrase of the first (ca. 2 typewritten pages) for publication in journals which were not prepared to accept the longer version. Some journals suggested for publication were:

<i>Angewandte Chemie</i>	(?)
<i>Chemical and Engineering News</i>	(shorter version)
<i>J. Chemical Documentation</i>	(longer version)
<i>Chemische Weekblad</i>	(?)
<i>Chemistry in Britain</i>	(longer version)

It was also suggested that contacts be established with:

Association of Editors of European Chemical Journals
Director of Books and Journals Division of ACS
Editors of the various chemical societies

Naming of Organic Reactions

Members agreed that the proposal of Prof. BUNNETT for the naming of substitution reactions could be extended to include other types of reaction. The details of such a system were not, however, discussed in depth because it was felt that there was more to be gained by awaiting the response to the announcement and reports discussed above. It was agreed that the general paper (74.4.19) could be used as a basis for the reports, but the inclusion of isomer proportions in the nomenclature system was not recommended. It was stressed that the system of nomenclature adopted should be kept free from any mechanistic details.

Mechanisms of Reactions

Members were unanimous in their decision that the Commission should not involve itself in a discussion of the numerous mechanisms for reactions which had been proposed to date. It would then be in the position of having to arbitrate between alternative mechanistic proposals.

Members were also agreed that it would be virtually impossible to describe all the processes which occurred in chemical reactions by means of a nomenclature system based on that of MATHIEU *et al.* [*Angew. Chemie* **72**, 71 (1960)]. However, in view of the present confusion in the area of the symbolization of mechanisms, it was felt that the Commission could perform a real service by setting up a system for the naming or symbolizing of idealized MODEL reactions, which authors could use as a basis for the discussion of real systems. Each model would carry a definite name or symbol, but the formulation of a model did not imply that it was a good representation of the mechanism of any particular specific reaction and the nomenclature system could thus remain detached from ephemeral discussions of controversial cases. This system would be completely independent of the system used for the naming of reactions and should be capable of specifying the nature of the reactants, transition states, intermediates, and possibly the rate-limiting step. Again, it was the general opinion that it would be better to await reaction to the reports of the Commission before deciding on a definitive set of rules for such a system, but a few basic principles were suggested. The symbolization should be:

- (i) easy to type;
- (ii) easy to use in speech;
- (iii) capable of being expanded to specify detail, but convenient to use in skeletal form;

- (iv) capable of indicating the completion of step, *i.e.*, attainment of an intermediate;
- (v) capable of indicating the character of the intermediate (*e.g.*, R^+ , R^- , R^\cdot , carbene, arylene, *etc.*);
- (vi) able to accommodate electron transfer processes, electrocyclic reactions, coordination with metal ions, excitation to higher electronic states, singlet \rightarrow triplet interconversions;
- (vii) adaptable in the sense that certain mechanistic details could be glossed over, especially beyond the rate-limiting step;
- (viii) capable of indicating the site(s) of reaction.

Definitions used in Physical Organic Chemistry

Members expressed the view that this was an area to which the Commission could give its immediate attention, but it was first necessary to establish contact with other IUPAC Divisions in order to prevent overlap of the work involved.

J. R. PENTON

COMMISSION ON ANALYTICAL REACTIONS AND REAGENTS (V.I)

Paris, 7 May 1974

Present: Prof. R. BELCHER (Chairman), Prof. F. PELLERIN (Secretary), Dr. J. BARTOS, Dr. A. HULANICKI, Dr. M. KAPEL, Mr. F. J. REIDINGER, Prof. H. WEISZ (Titular Members); Dr. M. HARMELIN, Prof. J. INCZÉDY, Dr. M. PESEZ (Associate Members).

Minutes of Previous Meeting

The minutes of the meeting held in Munich during 23-24 August 1974 had been published in *Comptes Rendus XXVII Conference* (pp. 185-186).

Membership

Prof. WEISZ would complete his first four-year period of Titular Membership in 1974. The Chairman was unanimously asked to request that the Membership be extended.

Finalization of Report on Amine Groups

This report had been studied and accepted at the previous Commission meeting. It would be sent to the Secretariat for translation into English of that part of the text drawn up in French. The report would then be sent to the Analytical Chemistry Division Committee for approval.

Colorimetry and Fluorimetry of Carbonyl Compounds and of Steroids

The report prepared by Drs. PESEZ and BARTOS had been studied in detail and it was accepted by the meeting. Nevertheless, there were several points to be checked concerning the nomenclature of aromatic aldehydes. On the other hand, the Members of the Commission wished that for each functional group mention should be made of the accuracy for a method. After discussion

it was considered that this addition should not be included in the actual document. It was decided that this study could be carried out on a method concerning each of the functional groups studied or in course of study (phenols, amines, carbonyls, steroids). Assembly of the results would be the subject of a special report. The report would be sent to Associate Members of Commission V.1. They would be asked to send their comments directly to Dr. BARTOS before 74.7.1, who would carry out the necessary amendments and then submit the report to Prof. BELCHER. The two reports would be finalized at the 28 IUPAC Conference (Madrid, 1975).

Redox Indicators

Dr. HULANICKI had prepared a further report on redox indicators. Comments should be sent directly to him before 74.7.1, and after amendment the report would be recirculated. Its adoption was envisaged at the meeting in Madrid in 1975.

Expression of Results in Colorimetry and Fluorimetry

Dr. BARTOS had prepared a report on this subject. Remarks should be sent to him before the end of July 1974. After study and amendment, Dr. BARTOS would forward it to Prof. BELCHER by December 1974. The Chairman would decide whether it was necessary to organize a joint meeting with other IUPAC Commissions thought to be interested in this subject.

Acid-Base Indicators and Polyphenols

Prof. PELLERIN indicated that these two reports were in preparation. They would be sent to Members of the Commission during the course of the first quarter of 1975 and would be the subject of preliminary discussion in Madrid.

Indicators for Complexometry

A report was presented by Dr. HULANICKI. Preliminary comments should be sent to him by 74.10.1. A general discussion would be held in Madrid.

IUPAC-CEE Contract

Prof. PELLERIN indicated to Members of the Commission the inherent difficulties in the execution of IUPAC-CEE contracts. He informed them in particular that CEE had not yet received the comments of its own scientific experts on the methods which had already been sent by IUPAC under the terms of the annual contracts. CEE had been unsuccessful in organizing a meeting between its experts and the IUPAC Coordinating Committee for Analytical Methods for CEE in November 1973 and again in February 1974.

The 1974 contract required the provision of only seven methods which would be circulated to Members of Commission V.1 and the Food Section. Prof. PELLERIN made several points concerning the methods which Members of the Commission would shortly receive. Amongst these methods, the determination of organic chlorine in benzoic acid and benzoates was the object of an exchange of views. In the first place the method proposed in 1973 related to the determination of total chlorine after mineralization; because CEE requested research on organically-bound chlorine it was convenient to work likewise on the chlorides (inorganic chlorine). Prof. PELLERIN had prepared a method which would be circulated. The amount of organic chlorine would be calculated by difference between total chlorine and inorganic chlorine.

Dr. PESEZ indicated that the amount of organic chlorine (700 ppm) which figured in the standard drawn up by CEE was very high: the Pharmacopoeias were orientated towards a standard which was much more severe (300 ppm for chloride and 150 ppm for organic chlorine, giving 450 ppm total chlorine). This would be taken into consideration and would be mentioned in the final despatch of the method to CEE.

Other methods of the 1974 contract were discussed and the comments would feature in the report concerning the methods for the 1974 contract.

Any Other Business

The principle of method 16/73 of the IUPAC-CEE contract (Limit Test for Thiosulfate in Sodium Sulfite) had been studied in Munich. Under the bibliography (P. PASCAL, *Traité de Chimie Minérale* 13-2 page 1419 and 5 page 608) the reaction should be read as follows:



Date and Place of Next Meeting

The next meeting of the Commission would be held in Madrid during the 28th IUPAC Conference (1975).

F. PELLERIN

COMMISSION ON MACROMOLECULAR NOMENCLATURE (IV.1)

Santiago de Compostela, 7-10 May 1974

Present: Dr. K. L. LOENING (Chairman), Prof. P. CORRADINI, Dr. R. B. FOX, Prof. T. TSURUTA (Titular Members).

Minutes of Previous Meeting

The minutes of the meeting held in Munich during 25-29 August 1973 had been published in *Comptes Rendus XXVII Conference* (pp. 176-178)

Membership

Because of the heavy work load of the Commission Secretary, Dr. L. C. CROSS, and his unavoidable absence from the meeting, it was agreed to ask Dr. FOX to act as Secretary until the 28th IUPAC Conference (Madrid, 1975).

List of Standard Abbreviations (Symbols) for Synthetic Polymers and Polymer Materials

The updating of Tentative Nomenclature Appendix No. 12 (February 1971) was complete, and the manuscript for the definitive version to be published in *Pure and Applied Chemistry* would be passed to the Secretariat.

Basic Definitions of Terms Relating to Polymers

As Chairman of the Drafting Committee, Prof. TSURUTA presented to the Commission a revision (dated 15 March 1974) of Tentative Nomenclature Appendix No. 13 (February 1971). The Commission made some minor revisions in wording of the document of Prof. TSURUTA. In addition, substantive changes were made in the front matter and in some individual definitions of this document. Structures would be drawn according to the

seniority rules of Tentative Nomenclature Appendix No. 29 (November 1972). The Commission agreed that the amended document of Prof. TSURUTA would form the final version for publication in *Pure and Applied Chemistry*.

Stereochemical Definitions and Notation

The Commission discussed the revised document (dated 4 April 1974) from Prof. CORRADINI entitled 'Stereochemical Nomenclature of Polymers'. The outline for further revision of this document was agreed.

Future Work

Action on the following items was deferred until the next meeting:

- (i) Nomenclature of Regular Single-strand Organic Polymers (Tentative Nomenclature Appendix No. 29: November 1972)
- (ii) Classification of Polymers by Families (a Committee on this subject, chaired by Prof. N. A. PLATÉ, had not yet reported)
- (iii) Nomenclature and Symbolism for Copolymers (a preliminary document written by Dr. FOX was circulated to the other Members of his Committee, Prof. G. SMETS and Dr. W. RING, and also passed to the participants of the present meeting)
- (iv) Subsidiary Definitions of Terms relating to Polymers (Prof. TSURUTA had submitted a new list of subsidiary definitions to the Commission)
- (v) Nomenclature of Inorganic Polymers (a document on this subject was expected before the next Commission meeting from the Polymer Nomenclature Committee of ACS)

Date and Place of Next Meeting

The next meeting was planned to be held in conjunction with the 28th IUPAC Conference in Madrid in the summer of 1974.

K. L. LOENING

COMMITTEE ON PUBLICATIONS

London, 28 May 1974

Present: Prof. G. OURISSON (Chairman), Dr. L. C. CROSS, Dr. R. L. KENYON, Prof. A. PEREZ-MASIÁ, Prof. B. C. L. WEEDON (Scientific Editor). In attendance: Dr. M. WILLIAMS, Mr. P. D. GUJRAL (IUPAC Secretariat); and in part Mrs. S. M. CAREY, Mr. H. F. ONLEY, Mr. R. COLE (Butterworths).

Minutes of Meeting in Munich (23 August 1973) and Matters Arising

The minutes of the previous meeting of the Committee on Publications (see *Comptes Rendus XXVII Conference*, pp. 76-80) were approved. The following matters arising from the minutes were considered further:

- (i) Sales figures for 1973 from Elsevier in respect of the soft- and hard-cover editions of *Enzyme Nomenclature* 1972 were encouraging. Because of possible implications for IUPAC nomenclature books issued through Butterworths, the mounting sales of the soft-cover edition would be watched carefully.

(ii) Concerning *Argon* 1971, it was noted that the Executive Committee had decided that, for a trial period of 3 years, 75% of the royalties received from Butterworths would be given to the IUPAC Thermodynamic Tables Project Centre at Imperial College, London. The Committee on Publications reaffirmed its opposition to the granting of royalties to IUPAC bodies from which the publications had originated.

(iii) Dr. KENYON reported that there had been no great rise in demand for tapes of meetings of ACS (about 25,000 cassettes were being sold per annum). There was still difficulty in obtaining the backup (illustrative) materials, in good quality or even at all, once a meeting had finished. ACS would continue this programme, although it felt there was unlikely to be any major expansion. In some cases ACS had rerecorded lectures with a professional speaker after first reworking the material recorded initially. There had been some experiments elsewhere in USA with videotapes, in which only the most relevant parts of lectures were recorded.

(iv) Concerning the points made by IUPAC in renewing its publishing contract with Butterworths, the latter had undertaken to consult the Union before finalizing the price of books other than run-ons from the journal, which was controlled already by an agreed formula.

(v) The Executive Secretary reported that there appeared to have been some misunderstanding about the preparation of consolidated five year indexes. Dr. GRÜNEWALD had indicated by letter that he was not in favour of this suggestion. Drs. CROSS and KENYON also advised against preparation of such indexes, which in their experience were not marketable commodities.

The Secretariat was asked to ensure that all IUPAC publications were being abstracted and included in *Chemical Abstracts*. Prof. WEEDON suggested that reprints of the annual listing of IUPAC publications in the *Information Bulletin* might be made for sales promotion by Butterworths and by Crane-Russak.

(vi) Dr. GRÜNEWALD had reported by letter several examples of IUPAC news in *Nachrichten aus Chemie und Technik*, often under headings other than 'IUPAC'. He felt that the information made available by the Secretariat to editors could be improved in order for it to be used more widely and more frequently. Further consideration of this matter was deferred to the next meeting when it was hoped Dr. GRÜNEWALD could be present.

(vii) Butterworths had confirmed that a copy of *Pure and Applied Chemistry* was being sent to the Science Citation Index at the Institute for Scientific Information. A survey made recently by the Secretariat had confirmed that PAC was definitely being included in *Current Contents*. Dr. KENYON advised on the need for IUPAC-Butterworths to have a contract with the Institute for Scientific Information regarding the 'original article tear sheet service', which could adversely affect IUPAC sales.

Matters Arising with Butterworths (Representatives of Butterworths present in part)

(i) 1973 *Sales and Royalties*. The files for the meeting contained a summary of the royalty position for the year ending 31 December 1973, together with a statement of sales per individual title. After deductions for purchases by IUPAC of £2,439.96, the net royalty paid to the Union was £8,669.13. Prof. OURISSON emphasized that, for the first time in recent years, there had been a decrease in the royalties. This was attributable only in part to the lesser

number of issues of PAC produced in 1973 compared with 1972. Prof. WEEDON noted that subscriptions to the journal were not dropping significantly, but that sales of books were appreciably less, especially those not run-on from PAC. He suggested that an analysis be made to ascertain if 1972 had been a vintage year for additional publications and if there was any effect from the biennial cycle of IUPAC activities.

Because of a reduction in staff at Butterworths, Mrs. CAREY had been unable to amplify the annual statement of sales by titles as suggested by Prof. WEEDON at the previous meeting. Nevertheless, Prof. WEEDON continued to press for the additional information to be included in future statements. He asked also for the summary of the royalty position to show a breakdown of 'other publications' into additional publications and run-ons from the journal. In reply to a question from Dr. CROSS, Mrs. CAREY said that when Butterworths' computerization was improved within the coming year, it should be possible to provide IUPAC with sales data perhaps quarterly rather than once per year.

(ii) *Discontinuation of Symposia Run-Ons from PAC.* The Chairman reminded the meeting that *Pure and Applied Chemistry* was an unusual kind of journal. It covered the full range of chemistry, through reports of Commissions, nomenclature rules, and the main lectures at symposia sponsored by the Union. Therefore, in order to provide for those readers or organizations which did not wish to subscribe to the journal itself, arrangements were made to sell reports or symposia lectures run-on as bound books.

In view of the steady decline in sales over the past 2 years, Mrs. CAREY on behalf of Butterworths had proposed to discontinue hard-cover run-ons of symposia material, starting in 1975. Prof. OURISSON reported that this proposal had been considered briefly at a recent meeting of the Executive Committee, where it was thought that a much more detailed analysis was necessary before IUPAC supported discontinuation of symposia run-ons; also, dissatisfaction had been expressed with the effectiveness of Butterworths' promotion of IUPAC publications. Subsequently, the President of the Union had informed Butterworths that he was personally against the proposal; he had suggested the use of soft covers and limited print runs in future.

Prof. PEREZ-MASIÁ thought there could be an argument to retain symposia run-ons, because specialist libraries might wish increasingly to buy them in preference to paying the rising subscription to the journal itself. Prof. WEEDON noted that, although Butterworths might be losing money for the run-ons, the latter still contributed significant royalties to the Union. He wondered if the reminder letter to symposia participants about the availability of hard-cover proceedings would come better from the organizers than from Butterworths.

Mrs. CAREY provided additional data to the meeting which showed that, in addition to 'Chemistry of Natural Products', there had been a drop in sales in recent years also for the series on 'Coordination Chemistry', 'Macromolecular Chemistry', and 'Analytical Chemistry'. The drop in sales reflected increasing pressures on library budgets and book prices being too high now for sales to individuals. Mrs. CAREY preferred to direct her more limited publicity resources in future towards increasing the circulation of the journal. She said that the difference in price between soft- and hard-covers for the run-ons was negligible; also, Butterworths had already in 1973 started to reduce the print-run for symposia run-ons from PAC.

Prof. OURISSON suggested that symposia run-ons could be discontinued if the relevant issues of the journal itself were simply made available for sale

to those interested in the symposia material. This would have the advantage that a definite price (that of a single or double issue) could be set in advance of a meeting. Difficulties were that:

- (i) some symposia issues would also contain reports of Commissions of no interest to the purchaser;
- (ii) there would be cataloguing difficulties for libraries.

Regarding (ii), Prof. OURISSON thought that a loose-leaf title page could be provided for casual sales of journal issues, leaving librarians to decide if they wished to hard-bind the material. The suggestions of Prof. OURISSON were accepted by the Committee on Publications and Mrs. CAREY as a basis for evaluation by the Secretariat and Butterworths.

(iii) *Price and Frequency of PAC in 1975*. The Chairman reported that the increase in subscription rate per volume to £14.50, requested by Butterworths and agreed at Munich, had not been implemented by the publisher. Butterworths now needed an increase to about £20 to cover rises in costs of paper, printing, binding, and subediting since the beginning of 1972. However, Mrs. CAREY was only seeking a rise to £18.00 per volume in 1975. Sufficient material was scheduled for publication in 1975 to justify continuation of four volumes of the journal each year.

Prof. OURISSON suggested strongly that any review of style for text pages of PAC should also take into account possibilities for reducing costs of printing. These included:

- (i) 'miniprinting' for experimental sections and those comprising expanded discussion of noncentral points (see *J. Org. Chem.*);
- (ii) two-column format per page (see *Tetrahedron*);
- (iii) smaller diagrams and formulae (see *Chemical and Pharmaceutical Bulletin*);
- (iv) unjustified setting (proposed by Butterworths).

Mrs. CAREY agreed to ask the production adviser at Butterworths to comment on these ideas.

Dr. CROSS indicated that publishing costs in UK would continue to rise by at least 20% per annum for the next few years. The increase in subscription requested by Butterworths was therefore warranted, and further increases were inevitable. He doubted whether savings along the lines suggested by Prof. OURISSON would greatly counteract inflation. Costs were highest for typesetting and corrections (*i.e.*, the actual number of words) and for postage and collection of subscriptions. The Committee asked the Assistant Secretary (Publications), when writing to Symposia Editors, to stress to authors the need to be concise. Prof. WEEDON wondered if IUPAC, even for PAC, should move towards printing by photooffset directly from authors' manuscripts. Dr. CROSS emphasized that offset did not necessarily bring savings compared with typesetting, because costs of paper, production, and postage were generally higher; this view was confirmed by Dr. KENYON.

With some reluctance, the Committee on Publications decided to recommend for approval by the Bureau a rise in subscription to £18.00 per volume in 1975.

(iv) *Revised Style for Text Pages of PAC*. Following acceptance of the new cover design for PAC, proposals had been submitted by Butterworths for a more modern style for text pages. Except for any minor changes which would effect economies, the Committee decided to defer consideration of this matter.

The possibility of selling individual issues of the journal instead of producing symposia run-ons should first be evaluated. Without a need to produce the run-on 'books', there would be a strong case to introduce a two-column A4-format for PAC, and the text style could be modernized at the same time.

(v) *Report of Scientific Editor and Status of Publishing Programme.* Butterworths was in process of moving much of its operations out of central London into Kent (Borough Green). This had adversely affected the subediting effort on IUPAC publications, with only a single person available over the past 6 months instead of the previous three people. A serious delay in expediting the 1974 schedule for PAC and additional publications, forecast by the Secretariat at the start of the year but discounted by Butterworths, had proved true in practice. Not a single issue of the journal for 1974 had yet appeared. In view of considerable efforts to bring the schedule right up to date in recent years, Prof. WEEDON expressed great concern that the issues for 1974 might not be completed even by early in 1975.

Mrs. CAREY said that the move to Borough Green for IUPAC publications was now expected before the end of July. Delays in the drawing office were being overcome by placing work outside the publisher. A second person had now been appointed to assist permanently with subediting of IUPAC material: he had previous experience of journal work and would move to Borough Green. Mrs. CAREY still hoped to complete the issues for 1974 before the end of the year. The Secretariat was asked to collect the material for publication in the fourth volume for the year as soon as possible (papers from V Magnetic Resonance and II Physical Organic Chemistry symposia, and reports from Sub-Commission on Calibration and Test Materials).

(vi) *Series Title for Data Compilation.* In 1970 Dr. WILLIAMS had suggested that *Selected Constants—Oxidation-Reduction Potentials of Inorganic Substances in Aqueous Solution* might form the first volume in a new series of supplements to PAC devoted to fundamental data in chemistry. The Committee on Publications had decided to publish it as a normal supplement to the journal, but the situation was now to be reviewed. Details were presented by the Executive Secretary of other data compilations issued subsequently or in preparation by IUPAC. Dr. CROSS said that, although the *Stability Constants* series had been very successful, he had experienced some failures with data compilations. He felt that the future handling of such material lay in utilization of the computer, with or without printing. Dr. KENYON referred briefly to the US National Standard Reference Data System established in 1963 to produce critically evaluated reference data in the physical sciences. This data was now being issued as *J. Phys. Chem. Reference Data* by ACS and AIP for NBS; individual data compilations were reprinted for sale. This project had grown rather slowly.

(vii) *Review of Title 'Additional Publication'.* While the Committee was still not happy with the title 'Additional Publication' for symposia material not previously published in the journal, no satisfactory alternative had yet been proposed.

(viii) *Distribution of IUPAC Publications in North America.* Mrs. CAREY reported that the arrangements made in 1972 with Crane, Russak & Co. Inc. (New York) for distribution of IUPAC publications in North America had proved to be very disappointing. The Executive Secretary said he was concerned not only at poor sales in North America but throughout the world. Mrs. CAREY shared his concern in respect of Butterworths sales

promotion within Europe and she would be looking to see if the publisher was under-represented there. However, she was quite satisfied with the Butterworths agent in Japan.

(ix) *Sales of Final Nomenclature Reprints by Secretariat.* Butterworths had agreed to sell reprints to IUPAC at approximately half the normal charge, but was not yet willing to provide reproduction pulls free of charge. The Committee recommended that if stocks of reprints became exhausted, the Secretariat should simply make photocopies for further sales or itself reprint the material by photooffset.

(x) *International Thermodynamic Tables of Fluid State.* A report was considered by the Committee of a meeting held at Butterworths on 11 February 1974 to review the status of this series. Mrs. CAREY had been disappointed at sales of the first volume, *Argon* 1971. The print-run for the second volume, *Ethylene* 1972, had been reduced and a rather high price proposed. For the next volume (carbon dioxide tables) offset printing directly from computer output sheets had been suggested instead of using computer (punched tape). When Butterworths could be provided with the original output sheets for carbon dioxide, Mrs. CAREY intended to make a cost comparison between the two forms of printing. It was agreed to review the whole publishing project once the carbon dioxide tables were published, because these should attract greater interest than the two earlier volumes.

(xi) *Standard Methods for Analysis of Oils, Fats, and Soaps.* Mrs. CAREY said that loose-leaf supplements to the 5th edition (1964) were not a viable proposition from Butterworths' point of view. She would prefer to publish supplementary material in PAC as it became available, then to consolidate it into a separate publication at longer intervals. The Executive Secretary suggested that reprints of supplementary methods in the journal might be sold from the Secretariat, it being left to purchasers whether to convert them to loose-leaf form. A wider margin would be needed than that normally used in PAC, so that holes could be punched conveniently in the reprints. Subject to approval by the Section on Oils and Fats, these proposals were accepted by the Committee on Publications.

(xii) *Renewal of Contract.* In view of the fact that printing in UK was now becoming rather prohibitive, and because of general dissatisfaction at the performance of Butterworths, it was decided to recommend that the Bureau should put the IUPAC publishing contract out for tender before the end of 1974. The Committee was not urging that any change be made, but it felt tendering was a necessary business procedure to be adopted by the Union to ensure efficiency. Drs. CROSS and KENYON could advise on specifications for tendering by other publishers.

Publication Implications of Reorganization of Inter-divisional Committee on Nomenclature and Symbols

Dr. CROSS had expected there to be publication implications if the traditional 'tentative' and 'definitive/final' stages of issuing IUPAC nomenclature rules had been discontinued in favour of a single stage of recommendation. Although the use of these terms had been abandoned by the Bureau, the two-stage process was being retained by the Union.

Membership

A vacancy existed because of the retirement at Munich of Sir HAROLD THOMPSON as Chairman of the Committee on Publications. It would be a good

idea to have a list of potential candidates available if the President of the Union wished to fill the vacancy. Prof. OURISSON agreed to write a circular letter on the matter to the Members after the meeting.

1973 Income-Expenditure Account for IUPAC Publications

A publications statement for 1973 prepared by the Secretariat showed an excess of income over expenditure of some \$23,000. The Finance Committee had agreed that the statement should include a credit transfer from the general account to cover free provision of publications to IUPAC bodies. Plans to present the publications data more clearly in the 1973 general accounts had not been implemented by the IUPAC Banker. The Executive Secretary had been asked to ensure the plans were fulfilled no later than for 1974. This would enable the introduction in 1975 of a formal publications account with all relevant items separated from the general account.

Publication of Reports from IUPAC Bodies

(i) *Letter of 30 January 1974 from Analytical Chemistry Division.* The Secretary of the Analytical Chemistry Division had referred for the attention of the Committee on Publications two reports from a Commission in his Division. Some Members of the Division Committee had recommended that these reports be published in PAC in a shortened form and either in full in a specialist journal or the full report be advertised as being available from the Secretariat on request. Prof. WEEDON was strongly of the opinion that Commission reports must appear in full in PAC (or as an Appendix to the *Information Bulletin*). Failure to observe this principle could only undermine the present basis of the IUPAC journal. He suggested that specialist journals should draw attention to publication by IUPAC of a report or, if it was not published, to its availability from the Secretariat. There was no support for the suggestion of Dr. CROSS for the British Library at Boston Spa to hold the reports on deposit. However, the Committee agreed with the proposal of Prof. OURISSON for the Union to make an experiment on this occasion: a synopsis of each report should be included in PAC with casual requests for photocopies of the full material to be serviced from the Secretariat.

(ii) *Recommendations on Education in Biochemical Engineering.* This report from the Fermentation Section was, in the view of Prof. WEEDON, unsuitable for publication in PAC. He felt it should be treated as a working document for the Section to produce specific proposals which might be issued by the Union. The Committee agreed to accept the offer of the President of the Applied Chemistry Division to discuss the matter, on its behalf, with the Chairman of the Fermentation Section. Prof. OURISSON said that this problem raised the general question of how to ensure that such reports came to the attention of all appropriate university departments. He wondered if it was possible to insert a notice in university bulletins.

Publication of Material from 25th IUPAC Congress (Jerusalem, 1975)

A letter was considered from the Organizing Committee, offering the 6 plenary lectures for publication by IUPAC, but preferring to have the main

section lectures and the symposium lectures issued as a special publication of the *Israel Journal of Chemistry*. Prof. WEEDON expressed a wish for IUPAC to continue the experiments of 1971 and 1973, when the Union decided to publish all of the main lectures, in a series of special volumes, by photooffset directly from manuscripts supplied at Congress by the lecturers. However, in view of difficulties in collecting the manuscripts in 1973, the Executive Secretary advised against continuation of the experiments. The Committee asked Dr. WILLIAMS to reaffirm to the Organizing Committee the right of IUPAC to decide what it wanted to publish from its biennial Congress, and to request full details of the scientific programme so that a decision could be reached as soon as possible.

Progress with Synopsis Journals, Ultra-Micro Print, etc.

Prof. OURISSON tabled some samples relevant to this item. He was interested to know if these concepts had implications for PAC and other publications of the Union. However, it was clear from earlier discussions at the present meeting that serious consideration of the new concepts was not yet possible by IUPAC. Dr. CROSS expressed the belief that the concepts would be adopted more widely as inflation in publishing costs continued. He anticipated that conversion to a synopsis format would be introduced first for primary journals rather than for journals like PAC.

It was agreed to invite Drs. CROSS, GRÜNEWALD, and KENYON to prepare for the next meeting reports, with samples, on the new concepts and especially with evaluations of miniprinting (*J. Org. Chem.*) and of the synopsis format now operating in *Chemie Ingenieur Technik*. Also, the present range of IUPAC publications should be reevaluated. To assist the reevaluation, the Executive Secretary was requested to circulate to the new Members of the Committee, with the minutes of the present meeting, the reports provided by Drs. GRÜNEWALD and KENYON in 1972 and the account of the discussions by the Committee in London. Prof. OURISSON would try to arrange a preliminary meeting with Drs. CROSS and GRÜNEWALD early in 1975 or late in 1974, at no expense to the Union, to prepare the way for constructive discussion later by the full Committee.

Date and Place of Next Meeting

The Executive Secretary reported that the 28th IUPAC Conference would be held in Madrid during 2-11 September, 1975. The Committee on Publications decided provisionally to meet on 2 September.

G. OURISSON

SUB-COMMISSION ON SOLUBILITY DATA (V.6.1)

Montreal, 10-12 June 1974

Present: Prof. A. S. KERTES (Chairman), Prof. A. F. CLIFFORD, Prof. G. H. NANCOLLAS, Dr. C. L. YOUNG (Members); Prof. I. ELIEZER (Representative of CODATA); Prof. R. BATTINO, Prof. C. D. BATTY, Prof. H. L. CLEVER, Dr. L. EICHER, Dr. K. L. LOENING, Prof. P. W. SCHINDLER, Dr. G. K. SIGWORTH (Observers).

Status Report

Prof. KERTES outlined the history of the Solubility Data Project since its initiation at the XXVI IUPAC Conference (1971) in Washington. The

Commission on Equilibrium Data (V.6), recognizing the need to compile and evaluate solubility data in all physical systems, established an *ad hoc* Committee consisting of the Commission Chairman (Prof. D. N. HUME), Commission Secretary (Dr. F. J. C. ROSSOTTI), and Prof. KERTES, to undertake a preliminary study on the need for such a project; its priority relative to other possible undertakings; its feasibility, cost, and appropriateness as an IUPAC project; and the possibilities of cooperation with CODATA and perhaps other international or national bodies known or believed to be interested in the project. The *ad hoc* Committee submitted its first report at the interim meeting of the Commission in Toronto, June 1972. At that meeting the resignation of Dr. ROSSOTTI from the Committee was accepted and Prof. NANCOLLAS had been appointed to replace him. The Commission endorsed the preliminary report, and charged the Committee with the responsibility of formulating the project in more detail and instructed it to elaborate proposals concerning its mechanism of operation and its scientific scope. At the XXVII IUPAC Conference in Munich (1973), Commission V.6 endorsed the Committee's report, the actions which had been taken, and submitted the project as an official IUPAC project to be operated by Sub-Commission V.6.1 on Solubility Data. Subsequently, on the recommendation of the Analytical Chemistry Division, establishment of the Sub-Commission was supported by the Bureau and approved by Council in Munich. The Project was to be a joint venture of IUPAC, CODATA, and Gmelin Institut.

CODATA Task Group

After brief introductory remarks by Prof. KERTES on the nature of the IUPAC-CODATA partnership in the Project, Prof. ELIEZER, Chairman of the *ad hoc* CODATA Task Group, reported on the steps undertaken in the organization of the Task Group. The IUPAC proposal for establishment of the Task Group was discussed at the 17th Bureau Meeting of CODATA (January 1973), and Prof. ELIEZER was authorized to contact the various Scientific Unions in order to identify experts who were willing to serve on the *ad hoc* Task Group. It had been emphasized that the Task Group should have as wide a representation from other Unions as possible in order to ensure that the Project achieved a broad scientific basis and would be supported internationally. The following Unions had so far nominated representatives to the CODATA Task Group:

IUGG	—	Prof. D. DYRSSEN (Sweden)
IUPAB	—	Prof. H. GUTFREUND (UK)
IUPAC	—	Prof. A. S. KERTES (Israel)
IUGS	—	Prof. J. A. KITTRICH (USA)
AIPEA	—	Prof. J. A. KITTRICH (USA)
IUCr	—	Dr. R. A. LAUDISE (USA)
WFEO	—	Dr. L. EICHER (USA)

Some of these appointments were made only a few weeks before the present meeting, and the financial responsibilities between CODATA and the participating Unions had not been clarified as yet.

Prof. ELIEZER's report on the organization of the Task Group was followed by a detailed discussion on its future role, and the following resolutions were adopted:

- (i) The CODATA Task Group and the participating Unions, as well as the non-ICSU Unions in WFEO, could not accept operational responsibili-

ties in the Solubility Data Project. It seemed impractical that scientists other than chemists or chemical engineers could be engaged in the actual scientific work of compilation and evaluation. This did not mean, however, that professionals associated with Unions other than IUPAC would not be qualified to do the scientific work if they had a basic training and actual experience in chemistry (metallurgists, engineers in materials science, pharmacologists, oceanographers, *etc.*). On the other hand, it was imperative that Unions found among their memberships one, or perhaps more, experienced scientists knowledgeable in the fields relevant to the Project who were willing to give their expertise and intellect to stimulate the interdisciplinary character of the Project. The meeting thus charged Prof. ELIEZER to distribute among the Unions the whole information available concerning the project and requested that the representatives prepare memoranda outlining the needs and interests of the participating Unions. This information should be available well before the next meeting (Madrid, 1975), and circulated among the Members of the Sub-Commission for comment.

- (ii) Because it was recognized that the chemical information generated by the Project was of interest to all branches of science and technology, Prof. ELIEZER should attempt to enlist the participation of additional international organizations, such as IUB, IMA, IUPHAR. In order to assist Prof. ELIEZER in his efforts, a memorandum should be formulated which described the aim, scope, and importance of the Project in scientific terms, so that the interest of other Unions, *etc.*, could be ascertained and translated into practice. Such a memorandum should include the philosophy underlying the Project, specify the areas to be treated, and give examples of tables. An *ad hoc* working team consisting of Profs. NANCOLLAS and CLIFFORD, assisted by Prof. BATTINNO, Prof. SCHINDLER, Dr. YOUNG, and Dr. EICHER, was set up to produce the memorandum.
- (iii) The Meeting charged Prof. ELIEZER to undertake the necessary steps in order to clarify the position of CODATA and the participating Unions concerning the expenses involved in the meetings of the Task Group.
- (iv) Prof. ELIEZER would report on the present meeting to the Treasurer and Secretary of CODATA when he met them in Paris later that month and prior to the CODATA Executive Committee meeting in Yerevan (21 June 1974).

Guidelines for Compilers-Evaluators

Prof. KERTES informed the meeting on his activities which resulted in the existing preliminary drafts of Guidelines. Starting in 1972 he had approached several experts in the various fields relevant to the Project, soliciting drafts of Guidelines. In early 1973 three versions of the Guidelines for Gas-Liquid Solubility Systems were prepared by Dr. YOUNG, Prof. BATTINO, and Prof. CLEVER, and Dr. W. GERRARD (UK). There were considerable differences both in the approach and the specifics of the three versions. In December 1973 Dr. YOUNG, Dr. GERRARD, and Prof. BATTINO met in London and discussed the differences of their drafts. Dr. YOUNG was charged to prepare a revised version based on the conclusions reached at their meeting. That second preliminary draft was now presented for further discussion.

On the basis of the first preliminary drafts, Dr. SIGWORTH had prepared supplemental sheets of Guidelines for Gas-Liquid Systems at high tempera-

tures pertinent to metallurgical systems. These sheets were now also presented for further deliberation. By a similar mechanism of solicitation two drafts of Guidelines for Solid-Liquid Solubility Systems were prepared, one by Prof. CLIFFORD and the other by Prof. SCHINDLER. Both were presented to the meeting. Attempts to enlist the cooperation of experts in the rather complex field of Liquid-Liquid Solubility Systems were so far unsuccessful.

After a long and detailed discussion of the presented versions of Guidelines, in which both general and specific changes of wording were suggested, the following resolutions were adopted:

- (i) *Gas-Liquid Systems.* The second preliminary draft of Dr. YOUNG which was under discussion, would be revised by the author in view of the comments expressed at the meeting. The resulting third draft, to be prepared by September 1974, would be circulated for additional comments which would have to reach the author by November 1974. In addition, Prof. KERTES would solicit comments on the third draft from experts not associated with the Sub-Commission. A final version would then be prepared by Dr. YOUNG and presented for approval at the Sub-Commission meeting in Madrid. If approved, it would represent the official version of these Guidelines. That final version should reach the Members by May 1975. Dr. SIGWORTH would prepare the supplementary Guidelines specifically designed for high-temperature gas-liquid solubility systems. This material would be circulated along with the third draft of Dr. YOUNG, and would follow the procedure outlined above. The supplement was an integral part of the general Guidelines.
- (ii) *Solid-Liquid Systems.* Prof. CLIFFORD would produce by the end of September 1974 a much extended and revised draft of the general Guidelines for these systems. Prof. SCHINDLER's specific Guidelines on heavy-metal salt-water systems would also be revised and would be included as supplements for solubility systems, in which ionic equilibria must be considered for a thermodynamic evaluation of solubility data. Prof. KERTES would continue to solicit additional drafts of Guidelines in these systems by individual contact. It would be desirable to have at least two additional and independent versions of Guidelines for solid-liquid solubility systems before the Sub-Commission could be asked to take decision on an official version.
- (iii) *Liquid-Liquid Systems.* Prof. KERTES would continue in his efforts to find experts willing to prepare Guidelines for these systems.

Compilation and Evaluation

There was an extended discussion on the mechanism of the actual scientific work of compilation and evaluation. The main point under prolonged discussion was the scope of the compilation on any given system. The following resolutions were adopted:

- (i) *Compilers and Evaluators.* The basic concept was that compiler(s) and evaluator(s) would belong to the same research unit. While exceptions were possible, it was recommended that the senior scientist in the research unit served as the evaluator of the compilation done by one or more (graduate student or junior scientist) compilers in his group. It was essential that the evaluator be a recognized expert in his field.
- (ii) *Scope of Compilation in a System.* Initially, all available literature values would be extracted and data sheets constructed for any given source.

From these sheets the evaluator would select those which were in his opinion the most reliable. The final compilation would include data sheets so selected. It was to be noted that one data sheet listed the information from only one original (primary) publication. All compilers would be identified in the sheets.

- (iii) *Scope of Evaluation in a System.* The evaluation text, the critical survey, included references to all published data. It contained narrative comments of the evaluator as to why certain data were not tabulated in the compilation part (no data sheets were published on them), and why they were rejected. Equally, the evaluator would comment on why certain data were regarded as reliable. The critical evaluation would end by a table of best (recommended) values.
- (iv) *Refereeing.* In order to ensure the highest possible quality of the work done in the frame of the Project, a series of review procedures involving outside referees, evaluators, and Topic Editors would be established.
- (v) *Work Schedule.* Noting the preliminary status of the existing Guidelines it was decided that the actual work of compilation and evaluation should be started as soon as possible on all systems for which preliminary versions of Guidelines were already available. It was estimated that on assignment units which could be presently defined, the work could start later in 1974. The meeting recognized the fact that solubility data information might be more urgently needed in some areas of science and technology than in others. It charged Dr. EICHER to identify through WFEO channels and personal contacts with Drs. BARLOW and WILENBROOK those areas which should receive priorities. Similar instructions would be given to the representatives of all Unions in the CODATA Task Group. Prof. ELIEZER had been charged to report to the Sub-Commission well before the next meeting.

Topic Editors

The duties and responsibilities of Topic Editors in general and the definition of the areas by their activities were discussed at length. Topic Editors, to be appointed according to needs, would have to:

- (a) recruit compilers-evaluators on specific assignment units
- (b) provide Guidelines and Model Data Sheets
- (c) provide blank forms for Data Sheets for compilation
- (d) provide model text for evaluators
- (e) engage consultants and referees for reviewing submitted evaluations
- (f) receive Data Sheets from the evaluators, and serve as the first reviewer for the scientific work
- (g) forward reviewed and edited Data Sheets and evaluations to the publisher

The meeting defined the following Topics and appointed the respective Topic Editors:

1. *Solubility of Gases in Liquids*

Topic: Solubility at room temperature and pressure below 2 Atm.

Topic Editor: Prof. H. L. CLEVER

Estimated number of systems: 2,000

2. *Solubility of Gases in Liquids*

Topic: Solubility at room temperature and pressure above 2 Atm.

Topic Editor: Dr. C. L. YOUNG

Estimated number of systems: 500

3. *Solubility of Gases in Liquids*

Topic: Solubility of inorganic gases at high temperatures, normal pressures (molten metals and alloys)

Topic Editor: Dr. G. K. SIGWORTH

Estimated number of systems: 500

4. *Solubility of Solids in Liquids*

Topic: Solubility of electrolytes (complex-forming heavy-metal salts) in water and aqueous solutions

Topic Editor: Prof. P. W. SCHINDLER

Estimated number of systems: a few hundreds

The Topic Editors had been authorized to use the preliminary Guidelines for distribution to potential compilers-evaluators, but should point out their status.

Computerization and Data Retrieval Systems

Prof. KERTES informed the meeting that his preliminary discussion with Prof. BATTY had resulted in the memorandum submitted by Prof. BATTY, which was among the documents distributed at the meeting. Prof. BATTY subsequently elaborated on his memorandum consisting of the following main points.

The computerization system which might suit the Project should be considered on the present plans that compiled Data Sheets would have the suggested format. These Sheets contained the names of the authors of the original communication (primary literature source), the names and symbols of the components, the experimental variables, the technique and method of instrumentation, and the numerical data themselves, possibly accompanied by graphs. In addition there would be auxiliary notes on the type of apparatus employed for the measurements, and evaluation of the error contained in the tabulated numerical data. An important addition to the Data Sheets would be the Evaluation Sheets, a narrative that summarized the work of all primary literature sources on identical systems, evaluated critically the numerical data reported, and tabulated recommended solubility data. The proposal under discussion was to make these data available to the user in two ways: (a) a set of published volumes in bound and/or loose-leaf form that could be updated by supplementary volumes, and (b) a computer-based information retrieval system for on-demand searches.

An early estimate would be some 5-30,000 Data Sheets to be maintained in machine-readable form. The programme package that would control and exploit this data-base should have the ability to construct and edit files, to reformat the records under instruction, to sort and print the records by any of a given set of characteristics and, of course, to retrieve any record according to subject key words. An equally important consideration should be given to the possibility of producing the printed volumes and the updating volumes from the computer-based system. This was fairly common nowadays (e.g., MEDLARS), but was more complicated than a simple machine-readable file for on-demand searches. It would be desirable to have an authoritative list of terms and names used in each of the areas worked out at an early stage

of the Project. This list need not be over-long and indeed would draw on much of the accepted terminology appearing on the Data Sheets. Prof. BATTY believed that the system as he saw it now should not present excessive difficulties, though probably much discussion was needed on the detail of the Data Sheets, the overall control of the project, and the dissemination service. From the point of view of information system design and maintenance, the Project seemed both worthwhile and feasible.

A long discussion followed, mainly as to whether existing systems for handling numerical data in science could be used and adopted for the specific needs of the present project, without necessarily attempting to develop a system for this project. The following resolutions were taken:

- (i) Profs. NANCOLLAS, ELIEZER, and KERTES, would contact organizations which were known or believed to have a developed computer system for treating numerical data and ask for assistance in setting-up the file system desirable for the project. The replies received would be forwarded to Prof. BATTY for evaluation and digestion. He would prepare his recommendations to be circulated before next year's meeting of the Sub-Commission. If needed, he would be assisted by Prof. NANCOLLAS.
- (ii) Prof. KERTES was charged to explore urgently with Gmelin Institut the implications of the possibility of production from a computer-based system. Gmelin's attitude was essential for the timing in setting up the system. If such a production procedure was acceptable and desirable from Gmelin's point of view, the system should be established as soon as possible, to be ready to accept the flow of Data Sheets expected to start reaching Gmelin in early 1976.

Publication

The meeting noted with regret that Dr. W. LIPPERT was unable to attend the meeting, so that the reaction of Gmelin to the various proposals discussed was unavailable. The following proposals under discussion needed urgent clarification with Gmelin:

- (i) The important policy decision taken (see *Compilation and Evaluation*) that the actual scientific work of compilation and evaluation started immediately on the systems for which Topic Editors had been appointed, implied that a publication scheme should be designed which would be able to handle a continuous publication of Data Sheets and evaluation texts as they became available. As discussed earlier (see *Computerization*), there was the possibility for making the Data Sheets and evaluation text available both in bound and loose-leaf volumes. The latter form of publication was, of course, designed to cope with a continuous publication procedure. It had been voiced, however, that loose-leaf publications were not very popular with librarians because of the additional work involved in handling additions of sheets to loose-leaf volumes. No suggestion was at hand for a mechanism for bound-volume publications.
- (ii) Gmelin was requested to comment on the possibility of producing the Data Sheets by computer-assisted phototypesetting, using punched cards or magnetic tapes. This was in view of the fact that the Project was exploring the need and feasibility for the establishment of a computer-based information retrieval system. In the probable case that the Data Sheets and evaluation narratives would indeed be filed in a computer system, the manipulation of computer-assisted photocomposition was expected to be relatively simple.

- (iii) Because printing of the Data Sheets was assumed to be done in the Federal Republic of Germany, perhaps through Gmelin's contract with Springer Verlag, the possibilities for using the techniques adopted by the US Government Printing Office should be explored already at this stage.
- (iv) A detailed and precise definition of the 'technical editing' ('Redaktion' in German) step was desirable in view of the various possibilities discussed earlier (see *Topic Editors*). Gmelin was expected to prepare the blank forms of the Data Sheets on to which the compilers would introduce the information in longhand and writing. It had to be decided as early as possible whether Gmelin could proceed from these sheets, or if not, in what form it wanted to obtain this product. It was the general feeling that indeed Gmelin would have to handle all additional steps.

Prof. KERTES was charged to discuss with Gmelin these problems as soon as practical, and to report to the Sub-Commission on aspects which affected the work of Topic Editors.

Solubility Data Centre

The establishment of a Solubility Data Centre was discussed in general terms. It was assumed that, among others, the Centre should maintain up-to-date bibliographic and reprint files in the whole area of interest to the Project, and should operate a distribution office to handle on-demand searches. It was found desirable to have such a Centre, and Prof. ELIEZER was charged to prepare a very detailed proposal on the establishment, operation, maintenance, and responsibility of the Centre. The document would be circulated for comment well before the meeting in Madrid.

Nomenclature and Coding

Dr. LOENING (Director of Nomenclature, Chemical Abstracts Service) addressed the meeting, emphasizing the importance of enforcing IUPAC recommended nomenclature. He stressed the importance of using terminology which was consistent internally, and of avoiding ambiguities in the compiler's Data Sheets. This was vital especially for a large variety of compounds used in the chemical and pharmaceutical industry, which were frequently known by their commercial or trade names. Lists of many nonproprietary names were published by various national and international bodies on a continuous basis. With reference to the possibility of a publication of Data Sheets in the form of loose-leaf volumes, it was essential that a consistent, comprehensive, and flexible coding system be worked out. Dr. LOENING expressed his willingness to examine the Data Sheets generated by the Project. A mechanism for this had to be established by the Topic Editors.

Financing of Project

Prof. KERTES described the financing mechanism of the Project. Two types of fund were needed. One, for the general operating expenses, mainly to assist Members of the Sub-Commission to attend meetings. This type of fund was difficult to obtain but some help was, and hopefully would be in the future, forthcoming from IUPAC, CODATA, and Gmelin. The second type of fund was needed to support, at least in part, the scientific work of compilers and evaluators. It was expected that individual scientists engaged in the Project would obtain their own financial support. However, it was the Project's

general policy to assist individual senior scientists in their application for funds. Some preliminary enquiries with US National Bureau of Standards, US Government, and with the Petroleum Research Fund, were encouraging in a sense that they expressed interest and willingness to consider individual proposals. Prof. KERTES emphasized that such applications must be submitted through official IUPAC channels in line with IUPAC Statute 9.42, which explicitly restricted the freedom of individuals to solicit funds on behalf of IUPAC.

Topic Editors would thus inform contributors to comply with these regulations. Proposals written in the accepted way of applications for funds, indicating the funding agency, should be forwarded to Prof. KERTES. Contributors were encouraged to submit such applications addressed to any organization, private, public, national or international in character, known or believed to have interest in supporting this type of scientific work. Direct preliminary enquiries to funding agencies were possible, but individuals should explicitly emphasize that they had no authority to solicit funds on behalf of IUPAC or CODATA.

Membership

It was decided that the Sub-Commission would recommend the nomination of Prof. CLEVER, Prof. SCHINDLER, and Dr. SIGWORTH to membership after receiving their written agreement to serve if elected.

Date and Place of Next Meeting

It was decided that the Sub-Commission would meet in conjunction with the 28th IUPAC Conference (Madrid, 1975). At least part of the meeting should be held jointly with the CODATA Task Group.

A. S. KERTES

APPLIED CHEMISTRY DIVISION COMMITTEE

Bedford, 10-11 July 1974

Present: Dr. H. EGAN (President), Dr. R. W. CAIRNS (Past-President), Dr. W. G. STOLL (Vice-President), Dr. A. J. COLLINGS (Secretary), Dr. J. A. EPSTEIN, Dr. A. F. LANGLYKKE, Dr. W. W. MEINKE, Dr. K. WEISSERMEL (Members). *In attendance:* Mr. R. W. FENNELL (Secretary, Analytical Chemistry Division), Mr. R. J. M. RATCLIFFE (IUPAC Secretariat).

Minutes of Previous Meeting

The minutes of the meetings held in Munich on 21 and 27 August 1973 (see *Comptes Rendus XXVII Conference*, pp. 215-218) were approved.

Meeting with UK Company Associates

Dr. EGAN reported on the informal meeting of the Applied Chemistry Division Committee with UK Company Associates in London on 9 July. A major problem was communication with industry, which needed to be convinced of the role which IUPAC could play. There was also a difficulty in defining the areas in which industry would like to see IUPAC work. The meeting had shown an interest both in the programme of the Division and Membership of it. Dr. EPSTEIN and Dr. STOLL thought IUPAC was an excellent way for bringing people together from industry. It was agreed that

the Applied Chemistry Division should play an important part in the involvement of industry with IUPAC and that a fuller meeting should be held to discuss the participation of industry in the programme of the Division in 1976.

25th International Congress of Pure Applied Chemistry

Dr. EGAN drew attention to the arrangements which had been made for the 25th IUPAC Congress to be held in Jerusalem during 6-11 June 1975. Dr. EPSTEIN said that the programme was of special interest to the Applied Chemistry Division and welcomed a suggestion, which he would pass on to Prof. Y. MARCUS (Organizing Committee), that a paper on the work of the Applied Chemistry Division should be included.

Division Programme

It was agreed that the Division should work towards the position whereby the programme of each Section was fully documented on a project basis, each project being defined carefully at the outset and progressed systematically on the basis of reports from the Section to the Division from time to time. A possible form of project statement was discussed, together with a progress form. Also, it was agreed that these forms should be made available to the Sections as soon as possible, for completion and return by the time of the 28th IUPAC Conference (Madrid, 1975).

Joint IUPAC-IUFoST Symposium (Hamburg, 29-31 August 1973)

Dr. EGAN reported that the Symposium volume on *The Contribution of Chemistry to Food Supplies* for which the Food Section acted on behalf of the Division, had now been published by Butterworths.

Reclassification of Sections of Applied Chemistry Division

Dr. EGAN reminded the Committee of the Bureau resolution at Munich and drew attention to proposals by the Committee on Statutes and Bylaws to reclassify Sections as Commissions and to IUPAC Secretariat comments on the probable implication of such a change. Sections would be replaced by Commissions, each having specific programmes, with individual Members responsible for progressing individual aspects. Also, Dr. EGAN referred to his letter of 23 January 1974 relating to Titular Membership and to the documentary summary of the Division Membership, 110 out of 127 of whom were 'trade and industry' rather than academic in orientation. Dr. LANGLYKKE commented on the need for infusion of new blood. He was concerned that the present lack of turnover of Section Membership would weaken the Applied Chemistry Division and stressed the need for the support of Company Associates. Dr. EGAN referred to views of Prof. H. SUOMALAINEN (Division Vice-President) and read the text of a cable received from him. Dr. CAIRNS drew attention to the fact that the present Bylaws stated that Titular Members of Sections and Commissions were elected for 4 years and could subsequently continue for a further 4 years: after 2 years of inactivity, this pattern could be repeated indefinitely. Under the new proposals a Titular Member could serve only for a total of 8 years; and that his total time within the Union on a particular Commission, either as a Titular or Associate Member, could not be more than 10 years. Possible Commissions, to replace the present Sections, might in the first instance be:

Air Quality
Fermentation
Food Additives
Food Contaminants
Oils and Fats
Pesticide Residue Analysis
Terminal Pesticide Residues
Water Quality

This would mean no increase in the number of Titular Members of the Division. On the proposal of Dr. CAIRNS, supported by Dr. LANGLYKKE, the Committee agreed unanimously to recommend a change from Sections to Commissions and to work towards this position from 1975: this would be in accordance with the changes proposed by the Committee on Statutes and Bylaws.

Analytical Aspects of Division Programme

Dr. EGAN reported that he had discussed with Prof. N. TANAKA (President of Analytical Chemistry Division) the analytical aspects of the Division's programme and welcomed Mr. FENNELL (Secretary of Analytical Chemistry Division) to the meeting. Mr. FENNELL presented a summary of his Division's programme and confirmed that the work of the two Divisions was largely complementary, but should be coordinated closely. Whilst it had been agreed that there was no serious overlap between the two Division programmes, continued close liaison with exchange of programmes was desirable and to this end a joint meeting of the Divisions should be arranged in 1975. Dr. EGAN referred to similar views expressed by Prof. D. N. HUME and Dr. E. O. HAENNI and reminded the Committee of the earlier interest in discussions on the principles of international collaborative analytical studies and the importance to applied chemistry of harmonization of these between the many organizations now concerned. The Committee also welcomed the prospect of exchange of programmes between all Divisions.

Environmental Aspects of Division Programme

Dr. EGAN referred to the report, previously circulated, which had been prepared by Dr. FREYSCHUSS and Mr. B. GÖRANSSON on Environmental Interests in the Applied Chemistry Division. The desirability of a separate Section (or Commission) on Environmental Questions was discussed but it was thought preferable, in the first place, to develop the programme on the basis of the Commissions discussed above, but with extended, more specific, terms of reference for the Commissions on Air and Water Quality to cover pollution abatement aspects. The potential overlap between the Air Quality Section and the Commission on Toxicology of the Clinical Chemistry Section was also discussed; this should be settled finally at a meeting of the Section which Mr. J. L. MONKMAN hoped to hold in Paris on 16-18 September 1974.

Dr. EGAN also referred to the communication, previously circulated, from Dr. R. N. JONES (President of the Physical Chemistry Division). It was agreed that it was desirable that programmes should be exchanged between the two Divisions and that the Physical Chemistry Division should be invited to send a representative to the joint meeting with the Analytical Chemistry Division which it was proposed to hold in 1975.

Dr. CAIRNS raised the question of the general subject, discussed at earlier meetings, and also raised in Dr. FREYSCHUSS' report, of the disposal of solid

wastes. It was agreed that the *ad hoc* three-man Committee, proposed and approved earlier, should be activated on the basis of discussions to be held between Dr. EGAN and Prof. S. J. PIRT (together if possible with a biochemical engineer to be nominated by Dr. LANGLYKKE). These would include the consideration of pollution abatement and solid waste disposal, together with 'terrestrial environmental' aspects of food and pesticide problems, including those currently under examination by the Division and its Sections.

Diversification of Programme

Dr. LANGLYKKE introduced his report on Diversification of the Programme of the Applied Chemistry Division. As guidelines for the selection of projects for study he suggested that:

- (a) projects should serve common purposes of science and industry, *e.g.*, those concerned with standards of measurement, definition, nomenclature;
- (b) the results should be of general utility, useful to all members of an industry group: and might as well be useful to government agencies, academic institutions, and the general public;
- (c) projects should not be concerned with features which are competitive with and within industry: they should not be concerned with process development, product identity and quality, product comparisons, except as such studies would be in support of the industry at large or would be designed to protect the consumer or useful to government agencies in establishing standards generally designed for protection of the public.

Areas suggested for the selection of individual problems for study included scientific and technological communication, resource development, environmental protection, industrial hazards, educational needs, and waste recycling (solid wastes management). Dr. WEISSERMEL drew attention to the need to define any overlap between the programmes of the Sections of the Applied Chemistry Division and the programmes of the other Divisions and to deal with this; the need to look into the training in chemistry, especially industrial aspects; and the desirability of looking into raw materials and new resources of these. He thought that the consideration of educational aspects could wait for the time being, although Dr. LANGLYKKE's report should be made available to the Committee on Teaching of Chemistry. In the following discussion, which also reflected the conclusions reached on analytical and environmental matters (see above), the proposals made by Dr. LANGLYKKE were generally adopted.

Report to Bureau

Following a summary of the discussion above on diversification of programme, environmental and analytical aspects by Dr. EGAN, the Committee considered a draft report to the IUPAC Bureau, previously circulated. It was agreed that the changes proposed should be initiated at the 28th IUPAC Conference in 1975, and that details (including programme details) should be worked out over the following 4 years.

Finance

Dr. EGAN reported that the 1974 Division budget had been cut by the Treasurer by 15-20% and that each Section had been asked to reduce its

costs in proportion. This had been done and Dr. EGAN thanked the Chairmen concerned.

Next Meetings

It was agreed provisionally that the Committee would meet on 2 and 7 September 1975 in Madrid, on the occasion of the 28th IUPAC Conference. If possible, the joint meeting with the Analytical Chemistry Division might be arranged for 2 September: Chairmen and Secretaries of Sections and Commissions would be invited to this meeting and to the Division Committee meeting earlier in the day. Dr. WEISSERMEL invited consideration of Frankfurt as a venue for any 1976 meeting of the Committee. It was agreed to bring this proposal forward in 1975, together with the possibility of associating the meeting with a wider discussion of resources development aspects with Company Associates.

H. EGAN

SECTION ON FERMENTATION (VI.2)

Vienna, 13-14 July 1974

Present: Dr. S. KINOSHITA (Chairman), Dr. J. C. HOOGERHEIDE (Secretary), Prof. A. FIECHTER, Prof. I. HORVÁTH, Prof. S. J. PIRT (Titular Members); Prof. H. DELLWEG, Dr. B. M. LAINE, Dr. A. F. LANGYLKKE, Dr. F. PARISI (Associate Members); Ing. H. WUTZEL (National Representative).

Minutes of Previous Meeting

The minutes of the meeting held at Munich on 22-25 August 1973 (see *Comptes Rendus XXVII Conference*, pp. 240-242) were approved.

V International Fermentation Symposium

IUPAC sponsorship of this Symposium was granted by the Executive Committee at its meeting in London earlier this year. Publication rights of the Union in respect of the specially invited lectures were waived. Prof. DELLWEG submitted to the Members of the Advisory Committee of the Section a tentative programme that was approved with minor changes. Papers would be divided over 23 scientific themes, covering the entire field of fermentation activity. Prof. DELLWEG would be Chairman with Prof. ZÄHNER (Tübingen) and Prof. SCHLEGE (Göttingen) as Vice-Chairmen. The Symposium would be held during 28 June-3 July 1976 at the Congress Hall in Berlin, the week after theACHEMA exposition at Frankfurt. Although some programme overlapping could be expected from a European Fermentation Symposium planned for October 1975 at Budapest and from an International Symposium on Continuous Culture in July 1975 at Oxford, it was decided that there was not sufficient reason to modify the proposed scientific programme for the V International Fermentation Symposium. Dr. HOOGERHEIDE was asked to notify Prof. AMMON of CIIAA, the sponsoring organization of the Budapest Symposium to that effect. A request had been received from the International Yeast Council as to whether a meeting on yeast technology could be run in conjunction with the V Fermentation Symposium as had been the case at the IV Symposium (Kyoto, 1972).

VI International Fermentation Symposium (1980)

Prof. T. K. GHOSE (India) was in contact with Dr. K. S. GOPALKRISHNAN of the Antibiotic Research Centre at Poona and with other personalities from industry as well as from government agencies in India in order to investigate the possibility of holding this Symposium in India. Within a few months he hoped to be able to come forward with definite proposals. It was considered still too early to investigate IUPAC sponsorship of such a meeting.

Cooperation with International Association of Cereal Chemists

Of the 32 Working Groups of ICC, Group 30, concerned with yeast quality evaluation, covered the main area of common interest. Group 30 had met at Vienna on 16 May 1974 and that meeting was attended by Dr. PARISI and Ing. WUTZEL. A copy of the minutes of that meeting was submitted. Reliable methods for determining the fermentative power and keeping quality of yeast would be studied by Subgroup 1. Because yeast quality could not very well be established using only one set of specific conditions, the project would be renamed 'Studies on the Properties of Yeast' instead of 'Yeast Quality Evaluation'.

Microbiological Aspects of Effluent and Water Purification

It was the general opinion of the meeting that the microbiological aspects of effluent and water purification were sorely neglected and that the Section could and should make a contribution, preferably in cooperation with the Water Quality Section of IUPAC. A first attempt to organize a jointly sponsored symposium on this subject (IUPAC-IAWPR) during the 1974 IAWPR conference in Paris (1975) had not been acceptable to IAWPR. It was decided that a Committee under the chairmanship of Prof. PIRT would investigate the possibility of organizing as soon as possible a symposium on this subject in cooperation with the Water Quality Section. Funds for such a symposium would have to be obtained from industry, governmental agencies, and/or United Nations agencies. As a start, a relatively restricted Gordon-type of symposium to survey the possibilities seemed to be in order.

Education in Biochemical Engineering

The report prepared by Profs. FIECHTER and PIRT had been submitted to the Committee on Teaching of Chemistry. Dr. LANGLYKKE would now submit it to the Applied Chemistry Committee, requesting Dr. H. EGAN as President for permission to publish it.

Glossary of Terms and Symbols used in Fermentation Literature

It was intended to include this topic in the programme of the V International Fermentation Symposium. Mr. W. K. BRÖNN would be requested to prepare a brief abstract of the compilation he had prepared as soon as possible for submission to the programme Advisory Committee of the Section.

SCP Standards for Protein of Microbial Origin

The final version of the report 'Proposed Guidelines for Testing of SCP Destined as Major Protein Source for Animal Feed' was scheduled for publication as a Technical Report appendix to the *Information Bulletin* (No. 12,

August 1974). It had been thoroughly reviewed by Members of the Fermentation and Food Sections and had been approved by the President of the Applied Chemistry Division. In the meantime, the PAG of the United Nations had published its Guideline No. 15, covering the same subject. Guideline 15 was far less specific than the IUPAC document, but was not at variance with it. The next step to be taken by the Section was to investigate SCP prepared from purified sulfite waste liquor ('Pekilo', a fungal product approved for animal food in Finland) and SCP prepared from methanol (ICI Ltd.). Contact would be made with the producers of these materials for residual potentially dangerous concentrations of substances not metabolized, such as sulfur dioxide in Pekilo or methanol in the ICI product.

Applied Chemistry Division Reorganization

Dr. LANGLEYKE informed the meeting that advanced plans existed to retitle Sections as Commissions. The Fermentation Section would become a Fermentation Commission. However, this would not result in any major change in the present programme of the Section.

Next Meeting

The next meeting of the Section would be for two days during the period 2-7 September 1975, in conjunction with the 28th Conference of IUPAC, to be held at Madrid.

J. C. HOOPERHEIDE

APPENDIX: Recommendations on Education in Biochemical Engineering

Introduction

1. There are at least two basic reasons to reconsider the existing situation in the field of bioengineering education:

- (a) The rapidly growing knowledge of structure and function of the living cell and the increasing understanding of how its activities are regulated give a rational basis for improvements and future progress in applications. New products, besides the chemical 'fermentation' products (wine, beer, spirit, *etc.*), are already produced on an industrial scale (antibiotics, amino acids, single cell proteins) or will be available in future in a broad spectrum (*e.g.*, enzymes). Biological cultivation methods will be more closely combined with those of biochemistry or organic chemistry (steroid transformation, enzyme engineering). Therefore, the practical application of living cells is called by expressions that differ from the classical term 'Fermentation' (Biochemical Engineering, Biological Engineering, Microbial Engineering, Technical Microbiology, Bioengineering, *etc.*).
- (b) In the past, science and engineering have been developed rather separately. However, a somewhat varied discipline named Bioengineering has been created by adding biological topics to curricula of chemical engineers.

Many institutions in Japan, UK, USA, as well as in other countries, have developed curricula for chemical engineers including biological topics at both the undergraduate and graduate level. However, results seemed not always to be satisfactory: 'The aim

of existing programmes has been to give the chemical engineer a modest knowledge of biochemistry and microbiology and an acquaintance with industrial practice in selected biologically orientated industries. The result is that the bioengineer so trained is seldom expert in any one field' (LIGHTFOOT, 1964).

On the other hand, engineering topics are ordinarily not included in biologically orientated curricula. There seems to be a strong tendency, at least in Europe, to include not only biological topics in chemical engineering oriented curricula, but also to offer some engineering disciplines to students whose background is principally biological.

2. The present situation is characterized by the fact that in analogy with Chemical Engineering, biological and technical knowledge must be combined. Under the pressure of more recent developments, there was an increasing need for a reorientation in the curricula designed for university students. Two letters dated 1969 to the Chairman of the Fermentation Industries Section expressed this need. The Section thereupon entrusted Prof. A. FIECHTER (Zürich) and Prof. S. J. PIRT (London) with working out suitable proposals as guidelines for improving the education at the academic level.
3. Study of the problem showed that the fundamental difficulties which stand in the way of a solution are:
 - (a) Great differences in the educational systems of the various countries.
 - (b) Differing comprehension of the terms used for designation of the field of activity of a bioengineer.
 - (c) Different understanding of the terms used to specify curricula.

Analysis of the situation led to formulation of the following three questions:

- How to define the different terms used to describe the activity of a biochemical engineer?
 - Should a special training in biochemical engineering also be included in undergraduate studies or should this training take place exclusively at the postgraduate level?
 - Is it possible to develop curricula in Biochemical Engineering from both streams, *i.e.*, from the engineering or a biological background?
4. To answer these questions a survey was carried out in 1971-72. Results of a Symposium held in Terre Haute (USA) in 1966 were distributed to experts in numerous countries (see Appendix I and Appendix II). Naturally, the greatest interest emanated from colleagues who are active in academic education. But discussions with participants of scientific meetings and seminars have also helped to clarify the situation. Finally, the results of the Round-Table Discussion at the first Symposium on Microbial Engineering in Mariánské Lázně (Czechoslovakia) in 1972 [see *Inf. Bull.* No. 44 (December 1972), pp. 91-94] are considered in the following recommendations as well as some articles which have been published earlier, *e.g.*:

R. M. ARTHUR: *Bioengineering Education Survey*. Rose Polytechnic Institute, Terre Haute. IV Bioengineering Symposium, 17-18 October 1966.

- E. L. GADEN: *Training in Bioengineering. Global Impacts of Applied Microbiology*, Stockholm, pp. 3665-3667, 1964.
- I. L. HEPNER: *Training for the Biochemical Industries. Adv. Appl. Microbiol.* **11**, 283-288 (1969).
- J. D. BRONZINO: *The Biomedical Engineer—The Role He Can Play. Science* **174**, 1001-1003 (1971).
- D. J. HOCKENHULL: *Progress in Industrial Microbiology*, **9**, 114-153 (1971).
- J. D. GOMEZ-IBANEZ (Ed.): *Int. Symp. on Chem. Education. Pure Appl. Chem.* **31**, 323-431 (1972).

Definitions and Comments

1. *Definition of the field.* First, definitions of the terms designating the field of science with its subdivisions were laid down. Our proposals, approved at the Kyoto Meeting of the Fermentation Industries Section in 1972 [see *Inf. Bull.* No. 44 (December 1972), pp. 27-29], were submitted for further discussion at the Round-Table Discussion in Mariánské Lázně. There were only a few comments or suggestions. Appendix III represents the final version. Acceptance of these definitions was reached relatively easily. It should be mentioned that the definitions as proposed in Appendix III do not necessarily imply the creation of particular and separated curricula for each subdivision (e.g., Biochemical Engineering—Food Engineering).
2. *Special training to be included in undergraduate studies.* There was little discussion of the question whether a special training should take place at the undergraduate level or not. It was argued that for many positions, the degree of Ph.D. is not a prerequisite but some specialized knowledge is advantageous.
3. *Minimum requirements for biochemical engineering curricula.* The results of the written enquiry, yielding 26 utilizable answers, are briefly commented on hereafter. They are the basis of a proposal for the definition of the two possible training routes, as formulated in Appendix IV. Answers were obtained from Czechoslovakia, Finland, Germany, Hungary, Japan, Poland, Sweden, Switzerland, UK, USA, and Yugoslavia.

Question 1: Do you think that the definition of the academic nature of the proposed curricula in the accompanying letter is sufficient (academic level, 4 years, leading to the degree of Biochemical Engineer)?

Result: Yes 88 % No 12 %

Comment: 4 years were found appropriate. Answers from UK were for 3 years, from Eastern countries (e.g., Czechoslovakia) for 4 or 5 years.

Question 2: Do you agree that both the chemical engineering as well as the more biologically orientated curricula may lead to the status of a *biochemical engineer*?

Result: Yes 80 % No 20 %

Comment: This was the crucial question. 20 % cannot see how to combine engineering and biology. There is a strong feeling that 'twisting' leads to a superficial training. This risk really exists if the undergraduate study is not to be unduly prolonged. It is,

therefore, a question of the extent of the subject in the various disciplines and of the intensity with which the subject is treated. There is general agreement that curricula should guarantee a sound background, allowing the student to work successfully in a particular field after completing his studies.

Question 3: Referred to an attempt to formulate minimum requirements of a standard programme. A list of Majors, Minors, and Options was enclosed with the questionnaire. It closely resembled the list produced in Appendix IV.

3a: Do you wish to include other topics in the basic training programme?

Result: 50% agreed to the proposals.

The following list enumerates the additional wishes.

Surface Chemistry, Interfacial Phenomena, Fluid Dynamics,
Macromolecular Chemistry and Biophysics, Statistics, Data
Processing, Thermodynamics and Kinetics
Sciences of Materials, Instrumentation and Analytical Methods
Principles in Electronics and Electricity
Impact of Technology on Society
Virology and Immunology
Cell Structure and Function, Ecology
General Microbiology including Taxonomy
Industrial Microbiology

Comment: These subjects can also be understood as partial fields of the disciplines listed in Appendix IV.

Question 3b: Do you wish to exclude topics, partly or completely?

Result: 12% of all answers contained remarks of minor importance.

Comment: Appendix IV was treated at the Round-Table Discussion in Mariánské Lázně. The extent of the list was in principle agreed. Important is the distribution of the weight given to the various disciplines, Question 4 gives a first clue for this.

Question 4: Do you think that the topics listed under Minors of each curriculum should be:

less than 10%

10-20% more than 20%

of the total time of studies?

Results: 2% were for less than 10%

50% were for 10-20%

more than 45% were for more than 20% of the total time (e.g., 30%).

Comment: The distribution of the Majors and Minors is difficult to define. Designation and extent of the subject can vary considerably in the imagination of the individual concerned. However, the impression is that much weight is attributed to the background subjects and to the applied disciplines. Nevertheless, the answers to Question 4 show clearly that the emphasis in the training should be with the fundamentals.

Question 5: Recommended Options

Results:	Effluent treatment	77%
	Ecology	62%
	Environmental Biology	73%
	Food Technology	58%
	Arts	19%
	Humanities	35%
	Management	9%

The results are self-explanatory. Arts should be omitted. Instead of humanities a foreign language might be listed.

Question 6: Desirability of industrial experience

Result: 50% of the answers were for 4 months
20% for more
25% for less
2% were for none during undergraduate studies.

Comment: Industrial experience seems to be a minor problem. Generally, proposals were for 2 or 3 months. Two periods of 6 weeks or two periods of 3 weeks were also mentioned. Much emphasis on practical work is given in Germany and Switzerland (6-8 months). However, it was mentioned that placement is critical due to the lack of suitable positions. Therefore, students accept any job provided salary is good.

Question 7: Dealt with a layout of a Course in Biochemical Engineering

Result: A mere description of single processes was proposed by only 3%
93% disagreed
3% found the inclusion of processes description in seminars a good solution.

— The list of topics to be included is as follows:

Kinetics of microbial growth (including batch, continuous, semicontinuous, synchronization methods)—Principles of biological regulation

Bioreactor design (mass- and heat transfer, mixing, aeration power input, scalingup, immiscible substrates)—Biochemical plant design—Process control (including automatic assay of chemical parameters).

Characteristics of cultures in bacteria, moulds, yeast, algae, and tissue culture—Enzyme reactors—Enzyme engineering—Membrane reactors—Work under sterile conditions—Metabolite detection—Vaccine production—Media design—Isolation, maintenance, and improvement of strains.

—100% were for a combination of lectures with laboratory work.

Comment: Much emphasis was given to laboratory training. Many Faculties have serious problems related to the inclusion of extended experimental work in undergraduate studies due to the lack of space and funds. However, quality of undergraduate teaching depends on extensive treatment of the topic, including experimental work. Submission of a thesis (Diplomarbeit) at the end of a 4-year study period was strongly recommended.

Further wishes related to other aspects:

The survey should be repeated every 5-10 years and be communicated to interested institutions. It should be determined how many persons with such a curriculum are required in Industry, Administration, *etc.* It appears that those responsible for training in the field need further information on the development of the subject.

Conclusions

We can draw the following conclusions from these enquiries:

- Academic training of experts is necessary for industrial processes where living cells or its parts are involved. The training should take about 4 years.
- Special training in Biochemical Engineering is to start at undergraduate level to meet the requirements of industry.
- Specialization should not be at the expense of an adequate training in the fundamental subjects. Postgraduate studies improve the knowledge in special subjects.
- Definition of terms is given in Appendix III.
- Training as a Biochemical Engineer can be developed from a fundamental study of either engineering or a biologically orientated subject. A suitable combination is given in the list of 'Minimum requirements' (Appendix IV).
- The intrinsic quality of the training is imperative. The receptive transmission of knowledge (lectures) has to be supplemented with experimental programmes. The experimental training in Biochemical Engineering is to be completed with an independent laboratory project.

Recommendations

- Approval of the 'Definitions' (Appendix III) of the 'Minimum Requirements' (Appendix IV) and of the 'Conclusions' by the Fermentation Section as 'Recommendations'
- Transmission of the 'Definitions' to the Applied Chemistry Division Committee of IUPAC with the recommendation for approval
- Publication of the 'Recommendations' in the IUPAC *Information Bulletin*
- The 'Recommendations' to be brought to the knowledge of:
 - suitable national or international organizations
 - institutes and persons who have cooperated

Appendix I: Definition of terms of the Arthur questionnaire (1967)

Medical Engineering is the application of engineering principles to control the environment so that it will be healthful and safe.

Agricultural Engineering is the application of engineering principles to problems of biological production and to external operations and environment that influence it.

Bionics is the study of the function and principles of operation of living systems with application of the knowledge gained to design of physical systems.

Fermentation Engineering is engineering related to microscopic biological systems which are used to create new products by synthesis.

Human Factors Engineering is the application of engineering physiology, psychology to the optimization of the man-machine relationship.

Appendix II: Bioengineering Education Survey (Answers from 110 American Institutions. Reported by R. M. ARTHUR, 1967)

	Medical Engg.	Environmental Engg.	Agricultural Engg.	Bionics	Fermentation Engg.	Human Factors Engg.	Other
Undergraduate or graduate	53 (48%)	74 (67%)	27 (25%)	25 (23%)	12 (11%)	31 (28%)	22 (20%)
Undergraduates only	14 (13%)	24 (22%)	22 (20%)	4 (3.5%)	3 (2.7%)	11 (10%)	9 (8%)
Graduates only	47 (43%)	71 (65%)	24 (22%)	24 (22%)	12 (11%)	29 (26%)	21 (19%)

Appendix III: Definition of the special fields of Bioengineering as understood by the Fermentation Section

Bioengineering			
<i>Biochemical Engg.</i>	<i>Biomedical Engg.</i> (including Human Factors Engg.)	<i>Food Engg.</i>	<i>Ecological Engineering</i> (Synonyms: Sanitary Engg., Environmental Engg.)
<p>Application of engineering to:</p> <ul style="list-style-type: none"> —production of antibiotics, amino acids, steroids, enzymes, nucleotides, and other cell products; active living cells; vaccines; alcoholic beverages; protein for food and feed —effluent purification —tissue culture of living tissues from plant and animal cells 	<p>Application of engineering to physiology, psychology and the man-machine relationship</p> <p><i>Medical Engg.</i> (as a part of Biomedical Engg.) is the application of engineering and biological principles in the development and provision of prosthetic devices and the application of engineering to instrumentation for application, particularly diagnosis</p>	<p>Application of engineering to food processing including fermented food (excluding production of raw material)</p>	<p>Application of engineering principles to control the environment so that it will be healthful and safe</p>

(a) Majors	Chemical engineering background	Biological background
Mathematics	<p>Linear algebra</p> <p>Differential and integral calculus</p> <p>Differential equations</p> <p>Statistics, theory of probability</p> <p>Data processing (analogue and digital computers)</p>	<p>Mathematics</p> <p>Linear algebra</p> <p>Differential and integral calculus</p> <p>Differential equations</p> <p>Introduction to statistics</p>
Physics	<p>(classical physics)</p> <p>Mechanics, heat, light, sound, <i>etc.</i></p> <p>including laboratory courses</p>	<p>Physics</p> <p>(classical physics)</p> <p>Mechanics, heat, light, sound, <i>etc.</i></p> <p>including laboratory courses</p>
Chemistry	<p>(principles of chemistry)</p> <p>Elements, stability and reactivity of chemical compounds</p> <p>including laboratory courses</p>	<p>Chemistry</p> <p>(principles of chemistry)</p> <p>Elements, stability and reactivity of chemical compounds</p> <p>including laboratory courses</p>
Organic chemistry	<p>Survey of organic chemistry</p> <p>Structure and reactions of organic compounds</p> <p>Principles and methodology of analytical chemistry</p> <p>including laboratory courses</p>	<p>Organic chemistry</p> <p>Survey of organic chemistry</p> <p>Structure and reactions of organic compounds</p> <p>Principles and methodology of analytical chemistry</p> <p>including laboratory courses</p>

Physical chemistry

Classical chemical thermodynamics

(Basic laws, activities, gas laws, thermodynamics of solutions of electrolytes)

Classical chemical kinetics

(Kinetics of gases, liquids and solids, elements of irreversible thermodynamics and phenomena of transport)

Principles of chemical spectroscopy

photochemistry and kinetics of excited states

Chemical engineering

Thermodynamics

Mass + energy balance (transport phenomena)

Chemical kinetics

Unit operations (size reduction, solids handling, mixing, separations, evaporation, gas absorption, distillation, leaching, crystallization, *etc.*) including laboratory courses

Process design

Technical, economic and social parameters

Analysis and synthesis of complex plant systems

Optimization studies

Exchange techniques

Reaction technique

Process control

Biology

General biology

(Cell structure and function, Principles in ecology and taxonomy of plants and animals, classical genetics, virology)

Physiology

(Plants, microorganisms)

Biochemistry

(including immunology)

Molecular biology

(including biophysics)

Microbiology

Genetics of microorganisms
including laboratory courses

(b) Minors (taking about 25% of total time of the curriculum)	
Introduction and principles:	Introduction and principles:
Biology	Chemical engineering
Biochemistry	(Unit processes, separation, classical thermodynamics and kinetics)
Physiology of cells and microorganisms	Process control
Biochemical engineering	Biochemical engineering
Genetics	Physical chemistry
Biophysics	+ minimum 1 month industrial experience
+ minimum 1 month industrial experience	

COORDINATING COMMITTEE FOR ANALYTICAL METHODS FOR CEE AND IARC

The Hague, 30 July 1974

Present: Prof. R. TRUHAUT (Chairman), Prof. F. PELLERIN (Secretary), Prof. R. BELCHER, Dr. H. EGAN, Dr. R. MARCUSE.

Minutes of Previous Meeting

The minutes of the Oxford meeting (see pp. 29-33) were adopted, noting that it was a meeting of the Liaison Group and not that of the full Coordinating Committee, which only met every 2 years at the IUPAC Conference. The present meeting was also only of the Liaison Group.

Report on Circulation of 1974 CEE Contract Methods

The methods had been sent by Prof. PELLERIN to Members of the Food Section and Commission V.1; Titular Members of this Commission had made a critical study of the methods at its meeting held in Paris on 7 May 1974 (see pp. 44-46). Prof. PELLERIN reported that he had received very few comments to date on the methods. The model questionnaire drawn up in Munich to accompany the methods had not apparently reached all Members. In these circumstances, the Liaison Group decided that a fresh circulation was necessary. Therefore, Prof. BELCHER and Dr. EGAN would contact the Secretariat again to send to all Members of the Food Section and Commission V.1 the 1974 Contract Methods accompanied by the questionnaire. The questionnaire should be returned to Prof. PELLERIN by 30 September 1974.

An examination of comments received to date:

Method 6/74 (Limit test for oxalate in calcium citrate—E233)

The method and text would be reviewed by Dr. EGAN.

Method 5/74 (Determination of organically bound chlorine in benzoic acid and its sodium, potassium, and calcium salts—E210-213)

This method gave rise to a long exchange of views. The determination of organic chlorine in benzoic acid and its salts implied the necessity of two determinations: total chlorine and ionic chlorine. It was thought necessary to draw the attention of CEE to the fact that the limits fixed for maximum amounts of organic chlorine (700 mg/kg for benzoic acid and 600 mg/kg for the salts) were perhaps too high according to several IUPAC experts. After enquiries it seemed that the following standards should be applicable:

ionic chlorine	300 mg/kg
organic chlorine	150 mg/kg
giving total chlorine	450 mg/kg

This conclusion would be sent to CEE for consideration. Meanwhile, the study would be continued by IUPAC experts and the method would be established compatible with the terms of the 1974 Contract. Prof. BELCHER thought it preferable to introduce nephelometric techniques.

Method 3/74 (Sulphur trioxide in sulphur dioxide—E220)

Prof. BELCHER thought that the method of SULLIVAN and WARNICK was not satisfactory. He said that a new method was in the course of study in his own laboratory. Under these circumstances, CEE would be informed that the method would be sent to it later. It was stressed that experimental work

carried out on analytical control methods by IUPAC was limited and could not automatically give results enabling the recommendation of an adequate method.

Finalization of 1974 Contract

The 10 methods of the 1974 Contract would be allocated as follows:—

- (a) Methods of 1974 Contract which would be the subject of a fresh circulation within IUPAC:
 - 1/74 — Limit of volatile fatty acids in lactic acid (E270)
 - 2/74 — Detection of α -naphthol in sodium *o*-phenylphenate (E232)
 - 4 and 5/74 — Bound organic chlorine (in fact total chlorine) and (and 10/73) Limit tests for chlorides in benzoic acid (E210-E213)
 - 6/74 — Limit test for oxalate in calcium citrate (E233)
 - 7/74 — Reducing substances in calcium lactate (E327)
- (b) Method in the course of study which would be sent to CEE at a later date:
 - 3/74 — Sulfur trioxide in sulfur dioxide (E220)
- (c) Method to be sent to CEE without further circulation:
 - Salicylic acid in *p*-hydroxybenzoic esters and their sodium derivatives (E214-E217)
- (d) Method already sent to CEE:
 - Nitrites in potassium nitrate (E252)
- (e) Nonvolatile matter in sulfur dioxide (E220—see below).

Nonvolatile Matter in Sulfur Dioxide

This method was listed in the CEE request for the 1974 Contract. After enquiries amongst specialists in gas analysis it was apparent that such a determination would not be of much interest. Dr. EGAN would, therefore, prepare a note on this subject which he would send to Prof. TRUHAUT.

Liaison with CEE regarding Future Contracts

Prof. TRUHAUT gave an account of the relationship with CEE. He regretted that despite repeated requests to the intergovernmental experts of CEE concerning methods already submitted by IUPAC, it had not been possible to obtain official comments on these methods. The joint meeting envisaged with IUPAC experts and those of CEE scheduled for February 1974 had not been organized by CEE. Prof. TRUHAUT recalled that publication of the methods by IUPAC could not be arranged before their publication by CEE. On the other hand, Prof. TRUHAUT informed the Liaison Group that CEE had given supranational status to its Scientific Commission which was now called the 'Scientific Committee for Human Food'. The initial meeting of the Committee was held on 21 June 1974 at Brussels. Prof. TRUHAUT had been elected Chairman and a work programme had been established. The next meeting would be held on 10-11 October 1974.

The extreme delay by CEE was accounted for by administrative difficulties due to the entry of new member countries into the Common Market and also to world monetary problems. CEE, conforming to the decision at the joint IUPAC-CEE meeting held at the beginning of November 1973 in Brussels, had not been willing to establish a contract for 1975. The cooperative action

of IUPAC-CEE to establish a programme in the course of this year was dependent on resolution of the problems and would probably lead to the establishment for purity criteria of new classes of additive.

Next Meeting

Prof. BELCHER indicated that certain research work of interest to the co-operative programme could be undertaken in his laboratory because of the presence of a significant number of postgraduate students. Prof. TRUHAUT thanked Prof. BELCHER and proposed that the next meeting should be held in Prof. BELCHER's laboratory in Birmingham at a date to be fixed.

F. PELLERIN

IUPAC COLLEAGUES DECEASED

We have been informed of the death of:

- UK* Dr. A. C. MENZIES (25 May 1974)—Commission on Spectrochemical and Other Optical Procedures for Analysis (1951—)
Sir ERIC RIDEAL (25 September 1974)—Commission on Colloid and Surface Chemistry (1961-)
Prof. C. L. WILSON (19 March 1974)—Commission on Microchemical Techniques (1951-1959)
- USA* Prof. E. E. SMISSMAN (14 July 1974)—Section on Medicinal Chemistry

REPORTS OF IUPAC-SPONSORED SYMPOSIA

IV CANADIAN WOOD CHEMISTRY SYMPOSIUM

Quebec, 4-6 June 1973

The Symposium was sponsored by the Canadian Pulp and Paper Association, Chemical Institute of Canada, and IUPAC. The attendance of 150 was 10% from Europe, 25% from Canada, and 65% from USA. The subject matter covered fundamentals of cellulose structure, oxygen pulping, and cellulose-polymer interactions.

Fundamentals

On the matter of cellulose structure there was much focus on new statistical methods for interpreting the X-ray structures of native and regenerated cellulose. For the former, the preferred conformation of the cellobiose unit was found to involve two intramolecular hydrogen-bonds (03 - - - 05) and (06 - - - 02) and a 'parallel' chain packing. Two independent studies by A. SARKO (Syracuse) and J. BLACKWELL (Cleveland) arrived at very similar conclusions on this matter. Both had used methods which were developed and described by the keynote speaker S. ARNOTT (Purdue), who showed how streaks on the X-ray patterns of polysaccharides, formerly ignored, could give valuable clues on elements of disorder in these structures.

The relation of conformation and chemical modification of polysaccharides and carbohydrates to enzymic reaction was discussed by D. A. REES (UK) and S. S. BHATTARCHAGEE (McGill). The former grouped all sorts of gelling polysaccharides together—hemicelluloses, carrageenans, and alginates—and showed how their helical conformations could lead to gelation through geometrical fitting, in terms of multiple helices, or ion binding or crystallization. The latter speaker gave a magnificent description of how enzymic methods can be used to define substitution in modified celluloses and how synthetic carbohydrate chemistry can aid in understanding the fine details of enzymic reactions.

Lignin received its share of attention. First from M. WAYMAN (Toronto) whose gel permeation chromatographic studies lead to a modular model for lignin, the basic module having a $\overline{DP} = 18$. Finally, H. R. GLASSER and W. G. GLASSER (University of Virginia) have resolved the complexity of lignin into a programmable model, which allows simulation of biogenesis and chemical reaction variables.

New Approaches to Pulping and Bleaching

Of eleven papers presented at this session, only three did not deal with the oxygen-alkali process, which seems to be the only candidate if pollution abatement demands a sulfur-free substitute for kraft pulping. However, the adoption of oxygen pulping would appear to involve a serious penalty, for unlike the kraft process large amounts of external energy may be required—to concentrate oxygen—and to compensate for the smaller energy derived from burning of the already highly oxidized byproducts.

Nevertheless, according to R. MARTON (Syracuse) a two-stage oxygen process can produce pulps nearly comparable in properties to *kraft*, while a one-stage oxygen process (D. M. MACKIE *et al.*, Montreal) can give products resembling sulfite. The greatest barrier of a one-stage process is that it requires

very thin chips (N. SANYER, Madison), but clearly a large number of variables remain to be investigated, such as the favourable effect of additives (e.g., Mn, iodide) or multistages such as proposed by I. PALENIUS (Finland). Several papers dwelt on the mechanisms of the probable reactions of carbohydrates and lignin in the presence of oxygen and alkali.

The keynote address by NILS HARTLER (Swedish FPL) provided a futurologist view on oxygen pulping especially in comparison to *kraft* and *sulfite*. If kraft mills continue to reduce their pollution level it is unlikely that a sulfur-free process will be needed. However, the simplicity of the oxygen process and the potential for smallscale operations may bring about some modest development by 1980 in spite of the obvious energy advantages of the kraft process.

Cellulose-Polymer Combinations

The keynote speaker took as his theme 'combine to serve' and indeed the session provided a series of examples on how cellulose fibres and synthetic polymers can be synergetically combined. Grafting of pulp fibres to improve water sorption was described by P. LEPOUTRE (Montreal), while R. B. PHILLIPS (Grenoble) showed how beating was accelerated and sheet strength improved by grafting polyacrylamide onto viscose or wood pulp fibres.

Two papers on encapsulation of wood pulps and already formed paper showed how the thermoplastic and water repellent characteristics of polyolefins can be married to cellulose by *in situ* polymerization using Ziegler-Natta catalysts. The fine dispersion of the catalyst in a paper matrix (R. H. MARCHESSAULT, Montreal) gives rise to a polyolefine with a unique morular texture which can impart unexpected advantages to the sheet, such as opacity and brightness. J. F. REVOL (Grenoble) showed how low quality fibres could be encapsulated and formed into sheets and heat-sealed to produce a composite with high wet strength and other desirable properties.

Physical mixing of synthetic polymers with native cellulose is an alternative to the *in situ* polymerization route to polymer blending. Likewise the irreversible adsorption of certain polymers bearing functional groups is an alternative to derivative formation. The latter was exemplified in the work of D. D. HALABISKY (Grenoble and Montreal), who showed how adsorbed polyethyleneimine effectively provided surface amine groups on cellulose. These were subsequently used to attach reactive dyes or neutral sizes.

R. H. MARCHESSAULT

INTERNATIONAL SYMPOSIUM ON CONTRIBUTION OF CHEMISTRY TO FOOD SUPPLIES

Hamburg, 29-31 August 1973

The Symposium was held at the Federal Chemical Institute of the University of Hamburg under the joint sponsorship of IUPAC and IUFOST in conjunction with Gesellschaft Deutscher Chemiker. The proceedings are now available as a Symposium Volume published by Butterworths (London) (see p. 129).

About 200 people attended the meeting, which was opened by Dr. E. LANGE (Chairman of Food Chemistry Group of Gesellschaft Deutscher Chemiker), who conveyed the greetings of the Ministry of Health of the Federal German Republic and stressed the importance of chemistry to the provision of present

and future food supplies. Prof. J. HAWTHORN (President-Elect of IUFOST) replied. The opening address was given by Prof. GEORGE F. STEWART (Department of Science and Technology, Davis, California), who spoke on international science and technology and international development. In his lecture he defined the relevant aspects of development and set out a basic philosophy for international development. He considered the various kinds of resources available, together with the various deterrents to development, and stressed the disadvantages of uncontrolled development, with special reference to the contributions chemistry and food science could make to development. These included enhancing the quality and quantity of raw food materials, improvement in technology of processing and preserving food and enhancing environmental qualities. Dr. HAROLD EGAN (Chairman of IUPAC Food Section) then described the current IUPAC programme in relation to food supplies, summarizing the work being carried out within the various Divisions of the Union which were relevant. The remainder of the meeting fell into three broad areas, the chemical modification of food, chemical contamination of food, and new proteins.

On the chemical modification of fats, Prof. J. W. E. COENAN (Netherlands) presented an interesting paper on the advances which were being made in the production of synthetic fats for human ingestion. Already a large proportion of edible fats are modified by physical and chemical means to increase the interchangeability of basic raw materials. He also gave some consideration to the nutritional aspects in the light of modern views on the effect of diet on health. Dr. MAGNUS PYKE (UK) continued the session with a stimulating presentation on the synthesis of proteins. Though it was possible to manufacture individual essential amino acids, the chemical structure of natural proteins is so complex and the molecular size so large that the probability of it ever being possible to produce significant quantities by chemical synthesis is remote. However, he did review the possibility of the production of polymers of intermediate molecular size in the form of proteinoids. The session was concluded by a paper by Dr. M. G. J. BEETS (Netherlands) on odour and molecular structures, which reviewed the types of interaction of various structure types and the sensitive parts of an organism which resulted in flavour sensation.

The session on the contamination of food was opened by Prof. J. C. AYRES (USA) with a paper on mycotoxins, in which he reviewed the various types of contamination which can occur and the factors which control them, together with the environmental conditions which have been found to enhance the formation of toxins. Dr. E. O. HAENNI (USA) considered progress in trace analysis for polynuclear aromatic hydrocarbons in food. The limit of detection was a few micrograms per kilogram, by methods which had been studied on a collaborative basis jointly by IUPAC and AOAC. Dr. A. E. WASSERMANN (USA) reviewed the advances in methodology in the detection of *N*-nitroso compounds in food. He also described some of their toxic properties and stressed the need for reliable methods especially at the very low levels found.

The final session, on proteins, was opened by Prof. J. HAWTHORN (UK), who reviewed the development of unconventional protein products over the past 20 years, including the generation of protein by direct photosynthetic means and the use of fermentation process to convert energy sources such as hydrocarbons and carbohydrates into protein. Dr. A. D. ODELL (USA) reviewed the advances which had been made in the structuring of protein materials using textile spinning techniques. Dr. N. S. SCRIMSHAW (USA)

discussed the work of the UN Protein Advisory Group on the appraisal of the nutritional significance of new proteins, with particular reference to the Group's Guideline No. 6, the recommendations of which should be met fully. In assessing the safety in use of new protein, Mr. J. McL. PHILP (UK) reviewed the type of problem which can be experienced with new protein sources. He stressed the need for the very careful evaluation of new proteins, especially as regards the type of contamination which can occur in natural protein sources. The session was concluded by Dr. W. MANSON (UK), who spoke on chemical possibilities for new proteins in relation to structural properties. He considered the physical, chemical, and biochemical properties of proteins and the manner in which these depend on the primary structure of the protein; and how these properties may influence the nutritional characteristics of the material. He described the modification of proteins to improve texture, in many cases a matter of overriding importance, and stressed the need for taking into account the nutritional requirements of proteins especially where they are needed in a predigested form, *e.g.*, for young children. He concluded that on the basis of knowledge already gained from the study of conventional proteins, it is possible to propose a research strategy for the production of proteins to meet particular requirements.

Simultaneous sessions dealt with submitted papers, covering a variety of subjects related to the main sessions, including the amino acid analysis of new proteins, the use of microwave heating in the production of soya milk, and the use of methanol fermentation to produce protein concentrate. Other submitted papers covered food additives and contaminants, unconventional proteins as aroma precursors in processed foods, heavy metals in corn food products, control nonenzymic browning reactions in food, and contribution of amino acids and peptides to food flavours.

H. EGAN

INTERNATIONAL SYMPOSIUM ON PLASMA CHEMISTRY

Kiel, 6-10 September 1973

The Symposium was held at the Department of Physics of the New University of Kiel, with the kind cooperation of Prof. W. LOCHTE-HOLTGREVEN. It was attended by about 130 delegates, including representatives from Austria, Belgium, Canada, DDR, Denmark, Federal German Republic, France, Hungary, Italy, Japan, Norway, Sweden, Switzerland, UK, USA, USSR, and Yugoslavia. The technical presentations included 6 invited papers (to be published in *Pure and Applied Chemistry* in 1974 (scheduled Vol. 39, No. 3), about 50 contributed papers and, a panel discussion.

The first and second days of the meeting included morning, afternoon, and evening sessions, followed by allday sessions on the third day. As a consequence of this hectic schedule, the beer-drinking evening organized for the third day by the local Arrangements Chairman, Prof. H. SUHR (University of Tübingen), was attended with considerable enthusiasm. Most of the delegates were nevertheless sufficiently recovered to attend the final sessions on 10 September.

The delegates were welcomed initially by the Meeting Chairman, Dr. J. R. HOLLAHAN (NASA Ames Research Center, California), on behalf of the Programme Committee and by Dr. R. N. JONES (National Research Council of Canada) on behalf of IUPAC.

A session on elementary chemical reactions in plasmas was introduced by Prof. A. T. BELL (University of California at Berkeley). An invited paper on chemi-ionization kinetics was given by Dr. A. FONTJN (AeroChem Research Laboratories, Princeton) and followed by several papers on the basic processes of electron attachment, electron production, ion-molecule reactions and recombination, largely in relatively cool, low energy plasmas. An invited paper by Prof. L. S. POLAK (Academy of Sciences, Moscow) discussed elementary chemical reaction kinetics in nonequilibrium plasmas, emphasizing the need for treating energy distributions of charged and uncharged species in detail for plasmas which cannot be meaningfully described in terms of temperatures.

The second session, on the chemistry of gas-phase and gas-solid processes under plasma conditions, was introduced by Dr. D. E. JENSEN (Ministry of Defence, UK Rocket Propulsion Establishment). An invited paper by Prof. E. MOLINARI (University of Bari, Italy) on homogeneous and heterogeneous reactions in plasmas of moderate pressure, described the successful application of basic principles of physical chemistry to several practical problems, including hydrogen atom production, synthesis of C_2H_2 and HCN, and metal oxide reduction. Several other papers in this session also contributed to a basic aim of the meeting—that of bringing together the interests of the fundamental research worker and the product-orientated synthesizer, with mutual benefit.

Prof. LOCHTE-HOLTGREVEN chaired the session on plasma chemical diagnostic techniques. Spectroscopic methods were reviewed by Prof. F. CABANNES (Centre National de la Recherche Scientifique, France) in an invited paper, and applications of microwave, mass spectrometer, electrostatic probe, and other techniques to a wide variety of plasma studies were described in contributed papers. Discussions arising from the papers in this session identified the need for better definition of plasma diagnostic methods—a task which the Plasma Chemistry Sub-Commission of IUPAC intends to take up.

Dr. C. BONET (Centre National de la Recherche Scientifique, France) introduced a session on engineering applications of plasmas. The invited speaker in this session (Dr. P. H. WILKS of TAFA, Bow, USA) discussed the future of plasma chemistry work from the industrialist's point of view, highlighting areas in which the special conditions of different plasma reactors could be particularly suitable. A number of contributing speakers gave examples of specific applications, Dr. W. H. GAUVIN (Noranda Research Centre, Quebec) describing an outstandingly useful plasma method of extracting molybdenum from its ore.

In the session on inorganic and organic syntheses under plasma conditions, chaired by Dr. HOLLAHAN, Prof. SUHR discussed mechanisms and uses of a number of organic syntheses under relatively cool plasma conditions in his invited paper. Other syntheses, both organic and inorganic, were described by contributors, the materials synthesized varying from organic polymers at one extreme to refractory inorganics like titanium carbide at the other.

The final panel discussion session was designed to provide a forum for international exchange of ideas concerning current and future activities in plasma chemistry. Of the four panel members, Prof. SUHR outlined future IUPAC plans for plasma chemistry cooperative efforts, Dr. I. G. SAYCE (National Physical Laboratory, UK) discussed government-industry-university interactions in plasma chemistry, Dr. V. IBBERSON (Polytechnic of the South Bank, London) made recommendations concerning standardization and reporting of plasma descriptions, and Prof. BELL reported on his

work on the international sharing of technical information. Vigorous comments on these contributions came from the attendees, providing useful input both for current work being organized by the Plasma Chemistry Sub-Commission and for organization of a proposed symposium on plasma chemistry planned for 1975.

It was generally agreed that the meeting had fulfilled a need in bringing together workers with both basic and applied interests in plasma chemistry. From the experience gained at this meeting, however, it was decided that future symposia would benefit from more time being allowed for discussion, as distinct from formal delivery of contributions, from better preparation of visual aids (especially for those gallantly speaking in an unfamiliar language), and from circulation of extended abstracts of papers prior to the meetings. The Programme Committee for the 1975 meeting will bear these points in mind, in preparing what it is hoped will be an even more successful gathering than the 1973 Symposium.

D. E. JENSEN

VI INTERNATIONAL MASS SPECTROMETRY CONFERENCE

Edinburgh, 10-14 September 1973

The latest in this series of triennial Conferences was held in the Appleton Tower of the University of Edinburgh. The Conference was organized by the Hydrocarbon Research Group of the Institute of Petroleum and was pleased to receive for the first time sponsorship from IUPAC, as well as support from the Royal Society and the mass spectrometry societies of eleven other countries outside UK. Representatives of these societies formed the International Committee which not only drew up the scientific programme, but also assisted in the task of refereeing the large number of papers submitted, to select those which could be accommodated within the time available. As it was, three parallel sessions were required for the presentation of 126 contributed papers as well as the 10 plenary lectures. The conference proceedings were published in June 1974 as *Advances in Mass Spectrometry* Vol. 6 (Editor: A. R. WEST, British Petroleum Co. Ltd.).

The Conference proved as popular as ever, being attended by some 520 delegates from 30 different countries (although it was regretted that the Soviet delegation was unable to come at the last moment). Interest in the lectures remained high throughout, with the main lecture theatre filled to overflowing on the final day. We were indeed fortunate that the Appleton Tower was equipped with closed circuit television, permitting overflow audiences to 'attend' the lectures in the theatres adjacent to the main one in use. The expansive Concourse, together with the neighbouring two floors, also provided an excellent and convenient setting for the exhibition; its closeness to the lecture theatres enabled delegates to examine in detail the most up-to-date products of the majority of the world's major mass spectrometer manufacturers. Minicomputers were associated with most of these instruments, both magnetic sector and quadrupole, and many mass spectrometers had gas chromatographs directly attached. It was a tribute to the manufacturers and the support from the University employees that the instruments worked so well under far from ideal circumstances. There was also a book display and a unique demonstration of computer matching of mass spectra against a library located in Maryland, USA. Delegates were invited

to submit their own 'unknown' spectra, through a teletype terminal in the exhibition and a satellite data link, to Maryland and achieve almost immediate printout of the names of those compounds in the library most closely resembling the 'unknowns'.

Prof. E. A. V. EBSWORTH of the Department of Chemistry, University of Edinburgh opened the Conference, and welcomed the delegates to Edinburgh. He was followed immediately by Prof. R. S. BERRY (University of Chicago), who gave a review lecture on 'Ionization Processes at Low Energies'. It has always been a feature of these Conferences that speakers of international reputation should give plenary lectures, which will act as keynote lectures for the immediately following contributed papers and which will also serve to bring together the specialists from diverse areas of mass spectroscopy. It may cause surprise that such a specialized subject should itself become fragmented, but experience has shown that it is very desirable for those working in one area to be educated in the thoughts and problems of very different ones: from such interactions the major advances often arise, so the plenary lectures bring together the physical chemist and the biochemist, the physicist and the analyst. These plenary lectures also provide valuable reviews of the state-of-the-art in various specialisms and as such make a useful contribution to the final published proceedings.

Prof. BERRY reviewed the present state of the theory of ionization processes at low energy resulting from photon, electron, and heavy particle impact. Direct and indirect processes leading to ionization were discussed in terms of the photoionization of molecular hydrogen. Chemi-ionization energy, storage modes and the relative roles of electronic and vibrational energy in autoionization processes were included in this review.

Prof. H. BUDZIKIEWICZ (University of Cologne) gave the plenary lecture on 'Biochemical Applications of Mass Spectrometry'. He selected research on carotenoids and nucleotides as illustrations of 'successes and difficulties, limitations and possible paths of future development'. The mass spectrometry of carotenoids can be subdivided into the identification of known compounds, structure elucidation of new compounds, and metabolic studies. Problems arise from their low volatility and thermal instability, but adequate attention to instrumental conditions produces repeatable spectra, even involving characteristic thermal decompositions. The spectra are sufficiently characteristic to provide structural information on unknowns, even of certain isomers, and typical fragmentation reactions have helped to elucidate the structure of, for example, luteoxanthin and diatoxanthin. The metabolism of green plants, involving violaxanthin, antheraxanthin, and zeaxanthin, has been studied with isotopic labels. Prof. BUDZIKIEWICZ discussed techniques for overcoming the involatility of nucleotides, by the formation of derivatives or by using field ionization or field desorption mass spectrometry. Sequencing of higher nucleotides is limited by molecular weight and complexity of fragmentations, but progress can probably be made by thermolysis or enzymolysis, followed by derivatization and field ionization.

Prof. J. D. CRAGGS (University of Liverpool) took as the subject of his review paper 'Mass Spectrometer Studies with Negative Ions'. He stressed the importance of mass discrimination and orifice sampling effects in studies on negative ion-molecule reactions, especially in relation to upper atmosphere studies, electrical discharges in gases, and combustion processes. He next considered threshold energies and the energy spreads of electron attachment processes, followed by reference to autodetachment lifetimes and studies of threshold excitations. Prof. CRAGGS concluded with a review of swarm

phenomena, with special reference to flowing afterglow and drift tube techniques, quoting results on high pressure oxygen negative-ion/molecule reactions.

Dr. R. E. HONIG (RCA Laboratories, Princeton) lectured on the 'Analysis of Surfaces and Thin Films by Mass Spectrometry'. He gave an in-depth review of four major methods—ion scattering spectrometry, secondary ion microanalysis, surface analysis, and ionized neutral mass spectrometry—used for analysis of surfaces and thin films. Theories of scattering and sputtering of particles from surfaces were presented and numerous types of instrument described. The scope and limitations of the various methods were discussed in some detail with reference to practical examples.

Prof. J. DROWART (Vrije Universiteit, Brussels) gave his review paper on 'Mass Spectrometric Studies in High Temperature Chemistry'. He discussed the identification of species, determination of thermodynamic properties of both condensed phases and gaseous molecules, and kinetic applications.

Prof. J. DURUP (Université de Paris Sud) spoke on 'Recent Progress in the Understanding of the Mechanisms of Ion-Molecule Reactions', concentrating on still existing problems. He first compared neutral-neutral and ion-neutral reactions, the latter requiring consideration of more than one electronic state of the system. Studies of the $H^+ + H_2$ and $Ar^+ + H_2$ reactions by the 'trajectory surface hopping method' were discussed, followed by more complex oxygen/nitrogen ion/molecule interactions via N_2O^+ . This led to a more general discussion of correlation diagrams and spin- or symmetry-forbidden reactions. Prof. DURUP described apparatus for the study of the lifetimes of the intermediate complexes, which could be lengthened by the complexity of the trajectories. The effects of the lifetimes of complexes and energy barriers on the trajectories on isotopic scrambling were finally considered, before brief reference to three other outstanding problems not treated in the review.

Prof. J. H. BLOCK (Fritz-Haber Institut der Max Planck Gesellschaft, Berlin) reviewed 'Ions on Surfaces, formed by Field Ionization or Ion Impact'. He considered ions that have been produced at or near surfaces. A brief introduction of principles was followed by a description of the atom probe field ion microscope (FIM), reactions in adsorbed layers on surfaces chemisorbed in structure, and field impulse methods. An interesting comparison was given between the capabilities of secondary ion and field ion mass spectrometry in the analysis of surfaces.

Prof. J. H. BENYON (Purdue University, Lafayette) lectured on 'The Determination of Ion Structure'. He emphasized that an understanding of structure was fundamental to the development of material sciences and went on to review the properties of ions and the traditional methods used for deducing some of these properties, viz, comparison of spectra, isotope labelling, and thermochemical measurements. Modern developments of these methods were discussed and other approaches described in some detail. Amongst these were approaches based on ion-molecule reactions, including ion cyclotron resonance experiments. Ion-photon interactions were discussed and the importance of the study of all aspects of metastable decompositions for the elucidation of ion structures was emphasized.

Prof. J. B. HASTED (Birkbeck College, University of London) spoke on 'Mass Spectrometric Monitoring of Ions in Plasma'. The measurement of the concentration of ions in a plasma is extremely important in the understanding of many of the processes that take place in laboratory-produced plasmas and in the upper atmosphere. Prof. HASTED outlined very clearly the basic physics

of ion extraction from plasmas, including sheath ion optical effects and the specification of an ideal plasma ion analyzer. His review indicated the great care that is needed to produce quantitative measurements of ion densities in plasmas using mass spectrometers.

Prof. T. L. ISENHOUR (University of North Carolina) spoke last, but far from least in a highly diverting and most instructive lecture on 'Information Theory and Mass Spectrometry'. His paper compared and contrasted some of the more traditional methods of interpreting mass spectra, *viz*, library searching, the Quasi Equilibrium Theory and computer aided interpretation, and then went on to suggest a new approach, *viz*, the use of Information Theory. The basic concepts of information theory were developed and its application to particular problems in mass spectrometry illustrated. In conclusion, some speculations were made with regard to the role Information Theory might play in mass spectral interpretation in the future.

To try to summarize such a feast of information is impossible: impressions are necessarily subjective and, with three parallel sessions even the most assiduous delegate must be very selective, so it would be unfair to choose for special mention lectures one had attended, to the neglect of those being given simultaneously elsewhere. Some points did stand out, though: 23 years after the first European mass spectrometry conference (Manchester, 1950) at least 26 of the 126 contributed papers were devoted to new instruments and techniques—the technology of the subject is far from static. Straightforward organic or analytical applications proved to be less popular, but there was great interest in biochemical applications. New techniques for the study of metastable ions produced not only revived interest in the pathways for ion fragmentations, but also increased concern for the energetics of fragmentation processes, a field promising much further study: continued interest in ion-molecule reactions was noted, with significant contributions from ion cyclotron resonance spectrometers. As minicomputers increase in power and availability, several authors described their use as spectral interpretive or library search instruments, as well as datahandlers, spectra producers, or selective ion monitors. Also during the programme, a sociologist examined the effect the personalities of some of the pioneers of mass spectrometry had on the development of the subject in its early days, an analytic approach which could be applied with interest elsewhere!

The social side of the Conference, with a banquet in traditional Scottish style and the opportunity to see parts of the delightful countryside around Edinburgh, was not neglected and gave valuable opportunities for delegates to renew acquaintanceships from opposite ends of the world. The City and Universities in Edinburgh were generous with their hospitality and goodwill. Delegates hope to meet again in Italy in 1976 as guests of the Italian Chemical Society.

A. QUAYLE

INTERNATIONAL SYMPOSIUM ON PORE STRUCTURE AND PROPERTIES OF MATERIALS

Prague, 18-21 September 1973

Pore structure plays a decisive role in the use of many materials in various areas of industry—chemistry, building, ceramics, metallurgy, agriculture, extractive industries, *etc.*, and its characteristics determine such important

properties as the mechanical and physical properties of materials, mass and heat transport, acoustic properties, electrical properties, problems of durability, *etc.* Therefore, the subject of pore structure of materials has been for a long time the one which attracted the attention of both academic research scientists and industrial engineers. In the past 20 years, a number of scientific meetings have been organized to bring together those interested in the fundamental and practical aspects of pore structure. The most significant occasions were the First and the Second Symposia on Methods of Investigation of the Structure of Highly Dispersed and Porous Bodies, held in Leningrad in 1951 and 1956; and the Tenth Symposium of the Colston Research Society on Structure and Properties of Porous Materials and the International Symposium on Surface Area Determination, both held in Bristol in 1958 and 1969. The International Symposium on Transfer of Water in Porous Media of the International Union of Testing and Research Laboratories for Materials and Structures (RILEM), held in Paris in 1964, and the Symposium on Flow Through Porous Media, held in Washington, DC, in 1969, should also be mentioned.

Recently, an opportunity for meeting of scientists trained in different disciplines, but all interested in pore structure, appeared again when the Czechoslovak National Committee of RILEM was invited to organize the International Symposium on Pore Structure and Properties of Materials under the joint sponsorship of RILEM and IUPAC. This Symposium was held in the buildings of the Faculty of Mechanical Engineering of the Technical University of Prague.

The Symposium was organized in Czechoslovakia by the Technical University of Prague-Building Research Institute, in cooperation with the Czechoslovak Scientific and Technical Society, Czechoslovak Silicate Society and its Working Group for Porosimetry, Czechoslovak Building Society, Czechoslovak Society for Industrial Chemistry, and J. Heyrovský Institute of Physical Chemistry and Electrochemistry of the Czechoslovak Academy of Sciences, as a part of the planned activities of RILEM Technical Committee No. 15: Pore Structure and Properties.

This Symposium was meant as an interdisciplinary meeting with two objectives: reporting and reviewing current progress, and bringing together workers from the 'pure' and 'applied' areas. The aim of the organizers was to accommodate under one roof people from various disciplines, and thus establish better grounds for the coordination of future research, to stimulate interdisciplinary activity, and improve the facilities for the application of knowledge of materials in their proper use.

The main problems of pore structure and its relationship with the properties of materials were grouped as follows by the Scientific Committee of the Symposium, the Chairman of which was Dr. J. M. HAYNES (Bristol, UK):

1. Pore Structure
 - 1.1. Models and geometry of pore structure
 - 1.2. Formation of pore structure
 - 1.3. Methods of determination of pore structure
2. Relationship between Pore Structure and Properties of Materials
 - 2.1. Mechanical properties
 - 2.2. Physical properties
 - 2.3. Durability

All working sessions were opened by general reports, followed by communications and discussions. General Reporters gave a critical analysis of the

individual reports published before the Symposium in the Preliminary Report (in two volumes, 1000 pages, by offset, in hard cover) as a basis of the discussions. An exhaustive survey of the present state of knowledge in the fields concerned and an outline of the perspective general lines of future research was also given in general reports.

The General Reporters for the individual topics of the Symposium were the world-known scientists:

- 1.1. A. E. SCHEIDEGGER (Austria)
- 1.2. K. S. W. SING (UK)
- 1.3. M. M. DUBININ (USSR), L. ZAGAR (FGR), and H. F. FISCHMEISTER (Sweden)
- 2.1. VL. ŠATAVA (Czechoslovakia)
- 2.2. A. V. LUIKOV (USSR)
- 2.3. M. MAMILLAN (France)

The languages of the Symposium were the official languages of RILEM: English and French, plus Czech and Slovak. All general reports, communications, and discussions were simultaneously translated into the mentioned languages. General reports with supplementary reports, communications, written discussions, and conclusions of General Reporters will appear in the Final Report (in four volumes, 1900 pages, by offset, in hard covers) in the course of 1974.

An exhibition of commercial instruments for pore structure analysis and an exhibition of books and scientific publications was arranged by the organizers at the Symposium Centre. Total number of participants in the Symposium was 384 from 27 countries (167 participants from Czechoslovakia).

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It is very difficult to give a comprehensive report about all general reports, reports, communications, and discussion contributions presented to such an interdisciplinary meeting of chemists, engineers, ceramicists, physicists, *etc.* Generally, however, it can be said that this Symposium was an interesting confrontation of different opinions on both pore structure analysis and the importance of pore characteristics for material properties. Its usefulness appeared probably most obvious in the case of the methods of pore structure analysis. The presentation of Academician DUBININ's and Prof. S. BRUNAUER's works can be mentioned here.

S. MODRÝ

V INTERNATIONAL SYMPOSIUM ON MAGNETIC RESONANCE

Bombay, 14-18 January 1974

The Symposium was held at the Tata Institute of Fundamental Research under the auspices of the International Society of Magnetic Resonance and the Association of Magnetic Resonance Spectroscopists (India). It was sponsored and supported by the Indian National Science Academy, Sir Dorabji Tata Trust, Tata Institute of Fundamental Research, IUPAC,

IUPAP, IUPAB and the Solid State Physics Laboratory of the Ministry of Defence, Government of India. The plenary and sessional invited talks are being published in the official journal of IUPAC, *Pure and Applied Chemistry* (scheduled Vol. 40, Nos. 1-2, 1974). The *Journal of Magnetic Resonance* has agreed to bring out special issues during 1974, incorporating the contributed papers of the Symposium.

The preparations for the Symposium were clouded by the Yom-Kippur war and the accompanying international oil crisis. The economic crisis in India magnified the uncertainty of a successful meeting and one should appreciate the efforts of the magnetic resonance workers, who finally ensured the success of the Symposium by turning up in large numbers with many interesting contributions. Of the 213 titles slated for presentation at the Symposium, 172 were actually presented. The Symposium was attended by 155 Indian scientists and 128 scientists from other countries.

The opening ceremony was held in the magnificent Homi Bhabha Auditorium at which Prof. A. K. SAHA (Chairman of the International Organizing Committee) welcomed the participants and traced the history of research in magnetic resonance in India. Prof. M. G. K. MENON (Director of Tata Institute of Fundamental Research) opened the Symposium and welcomed the delegates on behalf of the Indian National Science Academy and the host institution.

The scientific sessions of the Symposium started with the presentation of the International Society of Magnetic Resonance Award to Prof. HERBERT S. GUTOWSKY, whose contributions to the field of magnetic resonance were elegantly described by Prof. CHARLES P. SLICHTER. After receiving the award from Prof. FELIX BLOCH (Chairman of the Award Committee), Prof. GUTOWSKY delivered his address on 'Chemical Aspects of Magnetic Resonance', which was 'an unexpurgated historical synopsis of the early applications of NMR to chemical problems, with emphasis upon the importance of chance, serendipity, ignorance and faculty clubs'.

Except for the 9 plenary lectures which were delivered at joint sessions, the Symposium was conducted in three parallel sessions and the compact geography of the lecture halls contributed to the success of the parallel sessions. It was the general feeling that the plenary lectures were uniformly stimulating and provided a vista to the diverse applications of magnetic resonance. The high resolution NMR studies of partially oriented molecules, and particularly those dissolved in nematic solvents, were shown to yield molecular structural information (A. D. BUCKINGHAM). The stress was on recent applications to organometallic compounds and it was demonstrated how the metal-hydrogen bond length in transition-metal hydrides could be accurately determined in favourable cases. D. H. WILLIAMS described the general utility of NMR shift reagents and showed how by proper choice one could utilize them to study deuterium isotope effects and systems of biological interest. By ^{13}C -NMR spectroscopy one could separate the contact and pseudo-contact contributions in such complexes.

The applications of Fourier Transform Spectroscopy (FTS) and multiple resonance techniques have revolutionized the field of ^1H - and ^{13}C -NMR as applied to the study of complex organic molecules (W.V. PHILIPSBORN). The stereochemistry of *cis*-1,2-diiodonorborane and the structure and stereochemistry of a dimeric propellane, $\text{C}_{26}\text{H}_{22}\text{O}_4\text{N}_2$, have been determined by homonuclear INDOR spectroscopy. ^{13}C Fourier Transform Spectroscopy and ^{13}C - $[\text{H}]$ double resonance techniques have been utilized in the structural investigations of alkaloids, fulvenes, polyketones, organolithium compounds, and diene-tricarbonyl iron complexes.

One of the potentially most promising techniques discussed during the Symposium was Magnetic Resonance Zeugmatography (P. C. LAUTERBUR), through which proton distribution in space in living and nonliving systems can be mapped. LAUTERBUR uses a field gradient over the sample volume in the conventional high resolution NMR setup. Using image reconstruction techniques, it is possible to obtain the spatial distribution of liquids within complex objects or the spatial distribution of relaxation times, with a resolution of about 10μ .

C. P. SLICHTER described experiments on dilute Cu-X alloys ($X=\text{Cr, V, Mn, Fe, Co, Ni}$; impurity content of the order of 0.1 %). The copper atoms near the magnetic atom experience a Knight shift proportional to the conduction electron spin-polarization $\sigma(r)$. $\sigma(r)$ was measured in four neighbouring shells of copper. No discontinuity was observed in $\sigma(r)$ as a function of temperature through the Kondo temperature of CuFe. These observations—and others on single crystals of CuCo—give a new insight to the Kondo effect. R. VIJAYARAGHAVAN reviewed the recent work on cerium and samarium intermetallics. As a consequence of the mixing of higher ionic levels of Sm^{3+} due to the crystalline fields, the Knight shift (of X nuclei in Sm X_n systems) may exhibit anomalous behaviour as a function of temperature and the hyperfine field at a Sm site can be negative. J. ITOH reported the zero field NMR measurements on heavy rare earth metals and alloys by the spin echo method. The variations of the magnetic dipole and electric quadrupole hyperfine energies as a function of concentration and at the phase boundaries were determined.

S. R. HARTMANN discussed experiments involving spin and photon echoes in ruby and photon echos of Nd^{3+} ions in crystals of CaWO_4 , LaF_3 , and YAG. W. Low discussed how electron spin resonance can be utilized in mineralogy to understand the process of formation of minerals.

One of the parallel sessions was devoted mainly to the applications of magnetic resonance in biology. The most remarkable difference between the papers presented at this Symposium and at the previous one at Rehovot (1971), concerns the emergence at a widespread level of the use of modern technological advances in NMR for structural studies and studies of dynamic changes at the macromolecular level. These on the hardware side include: (i) FT-NMR spectroscopy and multiple resonance techniques, which have revolutionized the field of ^1H - and ^{13}C -NMR and enable the use of less abundant species like ^2H (H. H. MANTSCH) for structural elucidation; (ii) Rapid Scan Fourier Transform NMR (or Correlation Spectroscopy), which promises to be a less expensive competitor to the usual FT-NMR (E. D. BECKER); (iii) the use of π - τ - $\pi/2$ pulse sequence coupled with FT to determine the relaxation times T_1 and $T_{1\rho}$ for each individual nuclei whose resonance signals could be resolved and its use in studies of molecular motion and conformational changes in macromolecules (Y. ARATA); (iv) the use of high magnetic fields for studies in peptides (M. ANTEUNIS). On the software side we witnessed (i) the use of labelled ^{13}C precursors followed by ^{13}C -NMR in following biosynthetic pathways (G. G. GALLO); (ii) increasing use of shift reagents for assigning NMR spectra to help in the determination of primary and secondary structures of peptides (J. H. BRADBURY, M. ANTEUNIS).

K. WUTHRICH presented a vivid account of the status of ^{13}C -NMR in Hemes and Heme proteins with special reference to ^{13}C hyperfine shifts. The allostery of haemoglobin was also studied by magnetic resonance (K. GERSENDE). Several papers concerned with NMR determination of the

structure and conformation of proteins were presented (H. RUTERJANS, M. ANDORN, K. R. K. EASWARAN, J. L. MARKLEY, J. PARELLO).

J. CHARVOLIN demonstrated how proton nuclear magnetic relaxation could be useful in determining characteristic times of motions of molecules in soap-water and lipid-water systems. A. EHRENBERG has investigated the cytoplasmic membranes from *Bacillus subtilis* with nitroxide spin-labels which undergo restricted anisotropic rotational motion. Evidence was presented from NMR studies for a lipid core structure for egg yolk plasma lipoprotein (K. R. K. EASWARAN).

The measurements of ^{13}C linewidths and T_1 's of $^{13}\text{CO}_2$ and $\text{H}^{13}\text{CO}_3^-$ in solutions of native zinc-containing enzyme and the Mn^{2+} -substituted enzyme were utilized in determining the kinetic parameters of carbonic anhydrase as a function of pH and substrate concentration (S. H. KOENIG). Studies on binding of enzymes to substrates have also been investigated by ^1H -NMR studies (T. DRAKENBERG and J. L. MARKLEY).

S. H. KOENIG's work on magnetic field dependence of water proton spin-lattice relaxation rates of haemoglobin solutions and whole blood is very interesting. Through these measurements they have been able to show that water molecules can enter the red cells, bind to the haemoglobin, and exit from the cells in a time of microsecond or less.

The session on nucleosides and polynucleotides was marked by the intelligent use of the modern NMR techniques: FT-NMR studies on purine nucleotides and nucleosides by measurement of relaxation times (K. AKASAKA); ^1H , ^1H - ^{31}P , ^{31}P , ^{31}P - ^1H fast FT-NMR studies of 5'- β -nucleotides, adenosine diphosphoglucose, and uridinediphosphoglucose (R. H. SARMA); selective deuterium labelling and NMR studies of di- and trinucleoside, mono- and diphosphates (S. S. DANYLUK). R. TEWARI emphasized the need for a statistical approach to the interpretation of time averaged NMR properties and showed simulated structures of single stranded polynucleotides. G. B. SERGEEV has investigated the role of intramolecular interaction in nucleotides by NMR. D. J. PATEL outlined methods for assigning protons to particular base pairs in the proton NMR spectra of double stranded dioligonucleotides by ring current calculations.

The NMR investigation of proton relaxation by both T_1 and T_2 processes in a variety of model metalloporphyrin compounds has defined the factors governing spin relaxation in such molecules and has elucidated the motion of the out-of-plane metal ion relative to the haeme plane in high spin ferric porphyrine (G. N. LA MAR). The study of metal ion-guanosine monophosphate interaction by ESR of Mn^{2+} has indicated that both phosphate groups and guanine base are involved in the formation of the complex (S. K. PODDER).

The interaction of toxic chemicals like chlorinated hydrocarbons, organophosphates, etc., with proteins, enzymes, phospholipids, and model membranes, was studied by the changes in chemical shifts (R. HAQUE). The use of Karplus-type relations for vicinal NMR coupling constants in obtaining the conformation of molecules used as drugs was discussed (G. G. GALLO, G. CECARELLI, V. M. KULKARNI).

ESR studies of triacetoneamine *N*-oxyl (TAN) has shown that TAN reacts efficiently with sulfhydryl compounds and with reduced ascorbic acid and that oxygen forms a bridge between two TAN molecules. Such studies are expected to throw light on the mechanism of enhancement of radiation damage to anoxic cells by TAN (K. P. MISHRA). Reactions of electrons with simple amino acids and peptides in frozen alkaline and acidic

solutions have been studied by ESR. Evidence is obtained for the formation of amino acid dianions and deamination radicals (V. T. SRINIVASAN). The effect of EDTA on horse radish peroxidase in phenol ascorbic acid coupled oxidation (S. BHARATI) and the *in vitro* formation of ascorbic acid nucleic acid complexes (Y. D. SINGH) have been investigated by the ESR technique.

On the application side, the measurements of proton spin relaxation times by the spin echo method were utilized to differentiate between normal and malignant tissues (S. S. RANADE and S. R. KASTURI). Further, by the frequency and temperature dependence of proton T_1 , $T_{1\rho}$ and T_2 in porcine L. Dorsi muscle tissue, W. DERBYSHIRE has shown that the low frequency components of spectral distribution function are important in the relaxation behaviour of nonfreezable water in porcine L. Dorsi muscle tissue. The utilization of the pulsed NMR technique for rapid and nondestructive determination of oil in seeds was demonstrated by Indian agricultural research scientists (P. N. TIWARI).

About 100 papers presented in parallel sessions dealt with various physical aspects of condensed matter as studied by magnetic resonance techniques. These papers can be divided, in a broad sense, into the following categories:

1. *Electron spin resonance studies*

(a) γ - or X-ray irradiated crystals

Application of ESR and ENDOR to the study of colour centres was reviewed by C. RAMASASTRY. A number of ESR studies of the defect centres produced by X-ray or γ -ray were presented in crystals containing oxygen rich anions, such as chlorates, nitrates, sulfates, *etc.* (D. SURYANARAYANA, T. K. GUNDU RAO, C. S. SUNANDANA). The nature of free radicals generated in each case was discussed. R. SRINIVASAN discussed the results of ESR studies on X-irradiated antiferroelectric $\text{NH}_4\text{H}_2\text{AsO}_4$ and $\text{ND}_4\text{D}_2\text{AsO}_4$ and suggested a new model for the mechanism of antiferroelectricity in these crystals. ESR and ENDOR techniques have been applied to the study of the trapped hydrogen atoms in three crystallographic forms of $\text{Al}(\text{OH})_3$ (J. C. VODRINE).

(b) Doped impurities in diamagnetic systems

The relation between crystal symmetry and magnetic resonance was analysed (J. A. WEIL) from the following viewpoints: (i) maximum information obtainable about crystal symmetry, (ii) when does degeneracy occur, and (iii) knowing symmetry, what is the simplest way of measuring the tensors (g, hyperfine).

R. SRINIVASAN reviewed ESR studies on dialkyl thiocarbamates, dialkyl thiophosphates, and dialkyl selenocarbamates of copper. The observation of ^{33}S hfs in sulfur coordinated complexes has helped determination of the hybridization of the ligand orbitals. In Zn-diluted and Ni-diluted crystals of the diethyl dithiocarbamates, coupled pairs of copper ions have been observed and the exchange interaction has been determined to be ferromagnetic. Several contributions on Cu^{2+} , VO^{2+} , V^{4+} doped crystals and of Cu^{2+} in complexes provided information on the structure of the system under consideration, phase transitions, electronic spin density distributions on the impurity atoms and the ligands, *etc.* (P. VENKATESWARLU, B. V. R. CHOWDARI, S. SUBRAMANIAN, J. CHANDRASEKHAR, S. LAHIRY, S. K. GUPTA). Other impurities studied were Mn^{2+} (G. BACQUET), Gd^{3+} (D. VAN ORMONDT), Ni^{2+} (K. V. REDDY, T. RS. REDDY), and Tb^{4+} (G. L. DEL NERO). In one contribution an approximate spin Hamiltonian was constructed to describe the available experimental results on Fe^{3+} doped in tetragonal chalcopyrites, a ternary semiconductor (B. D. BHATTACHARYA). The ESR study of iron

impurity in GaAs reveals the change of Fe^{2+} to Fe^{3+} on heating at 900°C and the diffusion of zinc or cadmium is presumed to change Fe^{3+} to Fe^{4+} , resulting in the absence of an ESR signal (S. C. JAIN). M. BLUME presented an exactly soluble stochastic model which accounts for the ESR spectrum of CO_2^- defects in calcite.

(c) Other ESR studies

The ESR patterns of manganese(II) and iron(III) of nitrate and macro-molecular complexes in viscous solvents has revealed fine splitting and this is attributed to the fact that the zero field splitting anisotropies are not averaged out even at relatively high temperatures (L. BURLAMACCHI). The study of reduced active and inactive molybdenum catalysts has resulted in interesting correlations between the ESR spectra and the catalytic activity (G. MARTINI). The role of a particular radical ($g=2.003$) obtained during the catalytic process is studied with respect to its formation being an intermediate step in the catalytic oxidation of carbon dioxide.

The ESR studies of cobalt(II) porphyrins have been used as probes for the study of molecular complex formation with aromatic hydrocarbons (F. A. WALKER). The ESR spectra of bis [1-methyl 3-(2-chloro-6-methyl) phenyl triazine 1-oxide] cobaltate(II) has been analyzed to understand the electronic structure of the ground state (V. P. CHACKO). The ESR of $\text{Fe}(\text{CN})_5(\text{NH}_3)^{2-}$ in single crystals of $\text{Na}_2\text{Fe}(\text{CN})_5(\text{NO})$ at liquid helium temperatures shows the ground state to be distorted from the ${}^2\text{E}$ state of C_{4v} symmetry (B. R. MCGARVEY).

The electron acceptor properties of the nucleobases have been determined by the change of the radical concentration of an irradiated methylene blue-dimethylsulfoxide solution containing the nucleobases. The electron acceptor properties of the nucleobases corresponds to $\text{C} > \text{A} > \text{T} \sim \text{U}$ as has been calculated by PULLMAN. For studying the donor properties, an aqueous Cu^{2+} solution was used and the electron donor strengths are ordered as $\text{A} > \text{C} > \text{T} \sim \text{U}$ (W. LOHMANN).

CH_2 and CD_2 were generated by photolysis of diazirine and the ESR spectrum has shown that the triplet state is indeed the ground electronic state and that the molecule is bent with a bond angle of about 138° (R. BERNHEIM). The width of the exchange narrowed ESR line in antiferromagnets TiMnF_3 and TiMnCl_3 was observed (R. R. NAVALGUND) to be temperature dependent and exhibited anomalous behaviour near T_N . Metal to insulator transition was reported to have been observed (B. K. CHAKRAVERTY) in Ti_4O_7 by ESR techniques.

2. Nuclear magnetic resonance in metals and alloys

E. F. W. SEYMOUR reviewed NMR studies on liquid metals and alloys with reference to Knight shift and its variation with temperature (Korringa relation). He pointed out that the studies of electric quadrupole relaxation due to atomic motion hold promise of providing information on atomic short range order. An anomalous NMR line broadening was reported to have been observed (D. L. R. SETTY) in liquid Bi-Sn system. The Knight shift tensor was measured (V. V. ZHUKOV) in Cd-Mg and Cd-Hg alloys. The usefulness of this data in relation to the electronic structure of pure cadmium was pointed out.

S. K. SINHA reviewed the published data on acoustic NMR in metals. Theoretical methods for calculating the acoustic NMR absorption were also reviewed. Some metals exhibit $\Delta m_\text{I} = \pm 2$ transition, whereas several others do not. An electron-mediated nuclear spin-phonon interaction in metals

was considered (S. K. GHATAK) to account for such a behaviour. An analysis of acoustic NMR of spin 3/2 in cubic crystals was made (A. RAMAKANTH) using density matrix theory. Asymptotic charge density oscillation due to nonmagnetic impurity atoms and spin density oscillations due to magnetic impurity atoms in host copper and aluminium lattices were analysed (K. TOMPA) using Friedel and RKKY mechanisms. NMR line widths of ^{63}Cu in dilute Cu-X ($X = \text{Mn, Cr, Fe}$) alloys as a function of temperature and field have been studied (H. ALLOUL and P. BERNIER) and conclusions have been drawn relevant to the Kondo effect.

The technique of fast magic-angle specimen rotation has been used to reduce substantially the width of NMR spectra of ^{27}Al , ^{111}Cd , and ^{113}Cd in pure aluminium and cadmium. The isotropic Knight shifts were determined and the strength of the rotationally invariant Ruderman-Kittel indirect nuclear interaction in cadmium have been determined (W. S. HINSHAW). The temperature dependence of the nuclear magnetic and nuclear quadrupolar relaxation rates for liquid metal gallium has been investigated using the formalism proposed by SHOLL (N. C. HALDER). The s-d exchange model has been proposed for explaining the hyperfine field found in the binary and pseudobinary alloys, GdAl_2 , $\text{Gd}_{1-x}\text{Y}_x\text{Al}_2$, $\text{Gd}_{1-x}\text{La}_x\text{Al}_2$, LaAl_2 (M. M. BAJAJ).

3. NMR in nonmagnetic and magnetic insulators

I. TATSUZAKI reviewed NMR studies of phase transitions in dielectric materials. Studies of relaxation rates T_1^{-1} and the electric field gradients for various nuclei are most useful in understanding the dynamics of these systems. Anomaly in T_1^{-1} for protons in $(\text{NH}_4)_2\text{Cd}_2(\text{SO}_4)_3$ has been observed (P. RAGHUNATHAN) near T_0 . ^{51}V -NMR investigations on rare earth vanadates have indicated the presence of transferred hyperfine interaction possibly through a super exchange mechanism (S. GANGULI). A few papers were presented on NMR studies on hydrated crystals (C. R. K. MURTHY, J. RAMAKRISHNA). F. BORSA presented interesting results of nuclear spin-lattice relaxations in one dimensional paramagnets $(\text{CH}_3)_4\text{NMnCl}_3$ and $\text{CsMnCl}_3 \cdot 2\text{H}_2\text{O}$. In such cases, he argued, the relaxation rate diverges as $H^{-\frac{1}{2}}$, H being the applied field and this dependence was observed in the experiments. Zero field NMR studies on Rb_2CuF_4 were presented (L. C. GUPTA) and discussed with reference to the two dimensional nature of this system. A few papers dealt with ferromagnetic and antiferromagnetic resonances. C. M. SRIVASTAVA discussed ferromagnetic relaxation processes in magnetic insulators, while M. M. FARZETDINOV presented AFMR and NMR in weak ferromagnetics with a domain structure. The results of microwave magnetic resonance experiments in cubic FeGe were presented (S. HARALDSON).

4. Calculations of hyperfine magnetic fields

S. K. MALIK showed that the hyperfine field on the samarium nucleus induced by the paramagnetism of the 4f electrons may become negative because of crystal field effects, unlike the positive field in the free Sm^{3+} ion. T. P. DAS presented the results of calculations of hyperfine interactions in d-electron systems such as iron, cobalt, and a number of ionic ferric compounds. It was pointed out that in such systems, the exchange polarization plays a major role.

5. Nuclear quadrupole resonance

D. T. EDMONDS discussed in detail as to how nuclear double resonance techniques can be made use of in the detection of NQR in the region of frequencies as low as 50 KHz. He gave interesting examples of NQR by double resonance: ^{17}O (in natural abundance in organic solids and enriched ice), ^{14}N (in amino acids, purines, pyrimidines, and nucleosides, and in tetrahedral model compounds), and ^2D (in organic solids displaying fine structure due to D-D coupling). The applications of Fourier Transform Spectroscopy to NQR was discussed together with an experimental arrangement (E. A. C. LUCKEN). ^{35}Cl asymmetry parameters in a powder sample of mercuric chloride was determined using a frequency and phase locked NQR spectrometer (M. READ). A crystal structure and bond character study of 2,4-dichloroacetanilide by NQR was presented (P. VENKATACHARYULU).

The electric field gradient tensor at the Cl and Sb sites in SbCl_3 complexes was determined from the Zeeman split NQR spectra and a method for determination of the electric field gradient tensor for nuclei with integral spin from Zeeman split NQR spectra was presented (S. SENGUPTA). A theoretical method for determining the excitation spectrum of a spin one system with pure biquadratic exchange was presented (M. BARMA). T. P. DAS discussed the theory of nuclear interactions in metals (beryllium, magnesium, and cadmium) and ionic compounds (iron group).

6. Instrumentation

There were very few papers on instrumentation in the symposium. One could repeat here the development of correlation spectroscopy (Rapid-scan FT-NMR) mentioned earlier. Of particular interest was the paper on thermal detection of paramagnetic resonance (W. S. MOORE). This technique is eminently suited for the study of strongly coupled nonKramer ions.

Study of relaxation times to gain insight into molecular motions was the theme of several papers covering nuclear spin relaxation as well as electron spin relaxation. The proton spin-lattice relaxation times in $\text{CH}_4\text{-He}$, $\text{CH}_4\text{-Ne}$, and $\text{CH}_4\text{-Ar}$ mixtures studied as a function of temperature pressure and composition have been utilized to propose intermolecular potentials for these three systems (K. LALITA). In halogenated methanes in carbon disulfide the nuclear spin-lattice relaxation studies suggest spin-rotation being an additional relaxation mechanism besides the dipolar interaction (N. R. KRISHNA). The study of proton T_1 and coefficient of self-diffusion (D) in acetyl chloride, acetyl bromide, and acetone, in the temperature range 300-450 K has thrown light on the reorientational characteristics of the methyl group (P. K. MISHRA). The reorientation of the NH_3 group and the methyl groups (whenever present) at low temperature has been suggested by a study of proton magnetic resonance and relaxation study of eleven of the twenty amino acids encountered in proteins (E. R. ANDREW); correlation times, activation energies, and frequency factors characterizing each motional process, have been extracted. Reorientation rates of THF and water molecules in the clathrate hydrate of tetrahydrofuran have been studied (S. K. GARG). Similarly, the hindered rotation of the methyl groups has been reported for polycrystalline solid dimethylamine and dimethylamine clathrate dehydrate from 77 K up to the melting points of the respective compounds (P. RAGHUNATHAN). Selective proton T_1 measurements in the temperature range -15 - 80°C on substituted benzenes have indicated dipolar interactions to be the only effective relaxation mechanism, and it has been possible to separate the methyl group rotation from the overall rotation of the molecules in certain cases (J. SMIDT). The

effect of average librational motion of rigid molecules in the solid on the second moment of the NMR spectral line has been investigated and the intramolecular contribution has been corrected for these motions (M. POLAK).

The only paper on electron spin T_1 measurements was on a semiquinone ion in THF and acetonitrile; T_1 was found to be proportional to the radical concentration and followed the predicted viscosity and temperature dependence for nonhydrogen bonding solvents (S. K. RENGAN); the concentration dependence of T_1 was attributed to electron dipole-dipole interactions.

The ESR and Mössbauer of Ferredoxin from *Clostridium pasteurianum* has been interpreted by assuming spin-spin coupling between two clusters. (K. GERSONDE). A general expression for the Mössbauer line shape in the presence of radiofrequency perturbation has been obtained (B. KRISHNAMURTHY). The application of an external oscillating electric field whose frequency is equal to the dielectric relaxation or molecular reorientation frequency was found to change the saturation factor (R. J. SINGH). A new radiation occurring as a result of cross terms between the Zeeman-like radio frequency interaction and the orbit-lattice coupling is proposed to manifest itself as new side bands in the paramagnetic resonance phenomenon (K. N. SHRIVASTAVA).

The microwave optical double resonance technique has been utilized to assign the orbital symmetry of the lowest triplet state of 1,4 dihalobenzenes and for determination of the absolute signs of the zero-field parameters of excited triplet states (G. KOTHANDARAMAN). D. STEHLIK has proposed a mechanism for the optical nuclear polarization after light absorption in the singlet absorption region, and the polarization has been computed as a function of the external magnetic field and its orientation; and these predictions are compared with experimental features observed on crystals with partly deuterated or specific labelled ^{13}C -enriched host molecules.

The remaining papers presented at the Symposium can be classified to be of specific interest to chemists. Contact shift measurements coupled with magnetic anisotropy studies have been made on a novel system of spin $S = 3/2$ halogeno bis(*N,N*-diethyldithiocarbamate) iron(III). The contact shifts of the methylene protons vary linearly with the electronegativity at the halogen (Cl, Br, I) site (S. MITRA). The effect of *trans* ligand on ^{19}F resonance spectra of *trans*-(PPh_3) $_2\text{Pt}(\text{CF} = \text{CF}_2)\text{X}$, where $\text{X} = \text{SCN}^-$, NO_2^- , CF_3COO^- , etc., has been investigated (A. J. MUKHEDKAR).

Structural and conformational studies have been attempted using several of the modern techniques like liquid crystal NMR spectra, FT-NMR, etc. ^{13}C -acetylene, its effective structure, shrinkage effects, and apparent temperature dependent geometry (P. DIEHL), are conformation of 2,2'-bithiophene (A. C. KUNWAR), structure of pyridine and pyridine-*N*-oxide (C. L. KHETRAPAL), conformation of thietane, thietane-1-oxide, and thietane-1,1'-dioxide (R. MONDELLI), and nuclear magnetic shielding anisotropies in methyl fluoride (P. K. BHATTACHARYA), have all been investigated using liquid crystals as solvents. Here one should mention the observation that the temperature dependence of the contribution to T_1 and T_2 due to critical fluctuations in *p*-azoxyanisole can be described by a single correlation time due to critical fluctuations as given by the Landau-de Gennes theory (S. K. GHOSH).

The T_1 for methine carbons (^{13}C) in codeine, brucine, and reserpine, have been determined and the reorientational correlation times are estimated to be 3×10^{-10} to 2×10^{-10} sec. The fact that the relaxation rate of non-proton-bearing carbons is governed by geminal and in some instances by

vicinal protons allowed reliable assignments (F. WEHRLI). The vertical conjugation between benzene rings in monosubstituted (2,2) *p*-cyclophanes has been determined by ^1H - and ^{13}C -NMR studies (H. P. FIGEYS). ^{13}C -NMR of 1,4-polybutadienes catalyzed by π -allyl Ni trifluoroacetate systems show *cis-trans* sequence distribution (F. CONTI). The structure of a new indol alkaloid dimer, criophylline, has been determined by ^{13}C -NMR spectroscopy (G. LUKACS).

A complete analysis of the proton magnetic resonance spectrum of tetrahydrofuran at 60 and 100 MHz was presented (M. RICO). The structure of many isomeric pyrazolouracils have been predicted with NMR data (C. S. MAHAJANSHETTI). The utilization of conformational studies by proton magnetic resonance spectroscopy in establishment of the configuration of the Diels-Alder adduct was demonstrated (S. M. VERMA). Similar investigations have been carried out on the reactivity of *o*-hydroxyarylamides in alkaline solutions (P. M. NAIR). An NMR study of the syn-anti isomerism in *N*-substituted hydrazones of general structure $\text{R}_1\text{R}_2\text{NN}=\text{C}(\text{CH}_3)_2$, where $\text{R}_1 = \text{H}, \text{CH}_3$, $\text{R}_2 = \text{CH}_3, \text{C}_6\text{H}_5$ or *p*- XC_6H_4 ($\text{X} = \text{OCH}_3, \text{CH}_3, \text{Cl}, \text{Br}, \text{NO}_2$), was discussed in terms of specific molecular interactions (C. I. STASSINOPOULOU). The importance of chain branching and conformation on vicinal coupling in open chain aliphatic hydrocarbons and their mono derivatives was pointed out by G. SCHRUMPF. 2-Thiono-4-oxo and 2,4-dithiono-1,3-thiazanes with the methyl group in 5- or 6-position were studied to decide the conformation and the effect of aromatic solvents was used to assign the spectra (P. S. JOGDEO). Evidence was presented for hydrogen bonding in naturally occurring isomeric juglones (S. B. PADHYE). The ^{13}C -H coupling constants in substituted fluorobenzenes were found to increase linearly with the electron withdrawing power of the substituents and varied in the order: ortho < meta < para (R. D. SINGH); the ^{13}C -F coupling constants, however, did not show the same regularity, even though they depended on the substituent and its relative position.

A systematic study of ^{14}N -NMR spectra of conjugated *N*-heterocycles has provided a means of identification of azole ring systems. The ^{14}N chemical shift data could be accounted appropriately with the average excitation energy of the paramagnetic term while ignoring the contributions from the diamagnetic shielding term. The ^{14}N chemical shifts are found to depend linearly on the π -charge density at the nitrogen atoms as obtained from SCF-PPP-MO calculations (G. A. WEBB).

NMR studies of alkali resonances as well as ^1H and ^2D resonances in alkali radical ion pairs were discussed by E. DE BOER. From the ^1H and ^2D spectra the sign and magnitude of the hyperfine coupling constants, the electron spin, and the rotational correlation times could be determined. The alkali resonances furnish information about the sign and magnitude of the alkali hyperfine splitting constants, about ion pairing processes, and about the structure of the ion pairs in solution.

F. H. A. RUMMENS presented a new model for calculation of chemical shift medium effects by introducing an anisotropic potential in the statistical binary collision theory of RAYNES, BUCKINGHAM, and BERNSTEIN. The solvent effect on the thermodynamic and spectroscopic parameters in hydrogen-bonded complexes have been investigated by determination of the perturbation chemical shift of the hydrogen-bonded complexes (N. LUMBROSO-BADER). ^{13}C -NMR data were reported for aqueous solutions of aluminium perchlorate in organic solvents containing an $\text{X} = \text{O}$ solvating double bond when X is C (in amides) or P (in trialkylphosphates or phosphonates and in dialkyl hydrogen phosphites (J. J. DELPUECH).

Electron nuclear triple resonance of free radicals in solution has been studied (K. P. DINSE). The ENDOR investigation of hindered rotation in terphenyl anion radicals estimated the barrier to be 1.6-2.0 kcal. mole⁻¹ (R. BIEHL). ENDOR of bis-(3,5-di-t-butyl phenoxy)-methyl radical provided evidence for restricted rotation of both phenoxy and t-butyl groups (T. YAMAMOTO). The ENDOR of t-butyl-phenol nitroxide and 1,3,5-triphenyl-verdazyl were also assigned (T. YAMAMOTO). S. ARAVAMUDHAN reported the construction of a spectrometer for electron-nuclear Overhauser effect studies in solutions.

The kinetics of radiation damage in Teflon has been studied using ¹⁹F as a probe (L. N. MULAY). ESR was utilized to follow the variation in time of free radical concentration in organic substances (food products, etc.), and it was found that the water content influences the generation and recombination rate (G. FRITSCH). An elegant apparatus for estimating hydrogen and hydroxyl free radical concentration in premixed gas flames has been developed (E. L. SIMMONS).

This report does not claim to be complete, but does indicate the breadth of the Symposium. It is appropriate to end this report with remarks made by Prof. K. H. HAUSER at the closing session. 'In recent years the question has arisen at several occasions, is it still appropriate to have magnetic resonance conferences? It is true, that with the field growing and becoming more established, the emphasis is more shifted towards applications and one may argue that the results should be reported in conferences on the particular subject. As far as I am concerned, this conference has confirmed my opinion that magnetic resonance conferences are still useful, of course, only in addition to conferences on the different subjects. I enjoy hearing about the application of magnetic resonance to physics, chemistry, and biology and learning more about neighbouring fields, one of the main advantages being that it is easier to understand the results in a field somewhat more remote from one's own if one understands the method and hence the conclusions which can be drawn from experimental results. In addition to this fun, I think it is also useful for progress of science if people get a chance to learn about applications of their method in other fields because this can put new ideas into their heads about their own work. So my personal very subjective answer to the above question is that magnetic resonance conferences are still useful'. The VI International Symposium on Magnetic Resonance is to be held in Canada in 1977.

BALU VENKATARAMAN

II INTERNATIONAL MEETING ON BORON CHEMISTRY

Leeds, 25-29 March 1974

This conference, which was held at Boddington Hall on the campus of the University of Leeds, was sponsored jointly by IUPAC and the Dalton and Industrial Divisions of the Chemical Society (London). The plenary lectures are being published in 1974 in *Pure and Applied Chemistry* (scheduled Vol. 39, No. 4) and also issued as a separate book by Butterworths (London).

The meeting was attended by about 130 registrants, who illustrated the worldwide interest in boron chemistry, being drawn from UK, USA, USSR, Canada, Japan, Czechoslovakia, France, Germany, Hungary, Sweden, and Austria.

The delegates were welcomed to the meeting by Prof. N. N. GREENWOOD as both Chairman of the Organizing Committee and IUPAC representative. He expressed the feelings of those present in extending a particular welcome to Prof. H. J. EMELEUS, who acted as Chairman for the first session.

The first of the eight plenary lectures was given by R. SCHAEFFER (Indiana), who gave an authoritative account of recent advances in the chemistry of the boron hydrides, and emphasized the synthetic and structural approaches. He highlighted the preparation of $B_{14}H_{18}$, $B_{15}H_{23}$, and $\mu\text{-Fe(CO)}_4\text{-B}_6\text{H}_{10}$, and the recent structural determination on $B_{13}H_{11}$. The ambiguity in the proposed structure of B_5H_{11} was examined with reference to the 'unique' terminal hydrogen atom, and the results of a microwave investigation are awaited with interest.

The exciting developments in the chemistry of the metallocarboranes and -boranes were elaborated by M. F. HAWTHORNE (California) who, after giving a brief historical perspective, outlined the varied synthetic routes, developed mainly by his group, to the metalloderivatives. He emphasized the polyhedral expansion and contraction reactions as applied particularly to the species containing ten to fourteen vertices, and which are combinations of metal, boron, and carbon atoms.

The preparative theme was continued in the lecture by R. N. GRIMES (Virginia) who dealt with the metallocarboranes derived from the small carboranes, *i.e.*, those containing up to seven atoms of boron and carbon. Apart from the elegant syntheses of the direct and indirect insertion of metal atoms into the carborane frameworks, the rearrangement and structural studies on such systems were also emphasized.

The intermediate dicarba-nido-boranes formed the basis of an excellent lecture by S. HEŘMÁNEK (Prague), who dealt with the preparation of several new carboranes, such as $n\text{-C}_4\text{B}_{18}\text{H}_{22}$, which is new a carborane type consisting of two $C_2B_2H_{11}$ -units bonded by two three-centre bonds. General stability rules for the family of nido-carboranes were also proposed.

V. I. MATKOVICH (Carborundum Company, New York) gave a lucid account of the structural principles in refractory borides, and examined both the role of polyatomic groups and the various arrangements of icosahedral boron groups within metal borides. He showed that the understanding of the different structures of the lower borides is simplified if they are considered in terms of tetrahedra consisting of four metal atoms or two metal atoms and two boron atoms.

The industrial applications of boron compounds were presented by R. THOMPSON (Borax Consolidated Ltd., London), who emphasized that an inverse proportionality exists at present between industrial production and scientific interest in boron compounds. It is the four simple compounds—borax, boric acid, calcium borate, and sodium perborate—which account for 99% of industrial applications in tonnage over 2 million tons annually.

The varied reactions of allylboranes, especially those with unsaturated compounds, were discussed by B. M. MIKHAILOV (Moscow). Reaction pathways with acetylenes were outlined when cyclic boranes are often obtained, and other examples considered allenes and hydroboration reactions on the products of such reactions which yield boraadamantane compounds.

The final plenary lecture by A. G. DAVIES (London) considered homolytic reactions of organoboranes, where free radicals of various types interact with trivalent boron compounds such that an alkyl radical is displaced and substitution occurs at the boron centre. In an interesting and comprehensive discussion of this type of reaction other factors such as the kinetics and mech-

anisms of the reactions were discussed, and the application of ESR techniques to such studies was featured.

A book (copies available from Prof. N. N. GREENWOOD, School of Chemistry, University of Leeds, Leeds LS2 9JT, UK: £1.50 post paid) containing abstracts of 88 contributed papers was circulated to all participants before the meeting and this facilitated discussion; 43 of these papers were presented during the course of the scientific sessions.

There were also various social functions; on the opening evening Borax Consolidated Ltd. acted as host for a reception buffet, and a conference banquet was held on the penultimate evening. In between these two events a coach tour enabled the participants to enjoy the picturesque scenery of the Yorkshire moors.

The success of this meeting led those present to decide to shorten the time interval between such gatherings, and it is likely that the next meeting will be held in 1976.

M. G. H. WALLBRIDGE

II IUPAC CONFERENCE ON PHYSICAL ORGANIC CHEMISTRY

Noordwijkerhout, 29 April-2 May 1974

The Conference was held in the Netherlands at Noordwijkerhout, under the sponsorship of IUPAC and the Royal Netherlands Chemical Society. It was organized by a five-membered Dutch Committee supported by a four-membered International Advisory Board. The Conference was attended by nearly 200 participants, representing more than 20 countries from all over the world, including Australia, Canada, Israel, Japan, and USA from outside Europe. All participants were housed in the Conference Center 'Leeuwenhorst' surrounded by colourful tulip fields. With all delegates staying under one roof there was ample opportunity for effective scientific and social contacts.

The official scientific programme contained 7 plenary lectures (to be published in the IUPAC journal *Pure and Applied Chemistry*, provisionally Vol. 40, No. 4, 1974), interspersed with 38 contributed papers in parallel sessions. Each plenary lecture dealt with a particular aspect of Reaction Mechanism, which was the main topic of the Conference.

Prof. E. HEILBRONNER (University of Basel) gave a magnificently witty and original survey of UV photoelectron spectroscopy and its application to the study of electronic properties of organic molecules, thus elucidating the often complicated mechanisms of interaction between functional groups in such molecules.

Prof. G. G. HAMMES (Cornell University) discussed the mechanism of Enzyme Catalysis and Regulation with emphasis on methods and results of modern physical techniques used in the measurement of enzyme kinetics. Specific initiation of catalysis and regulation were discussed with particular reference to ribonuclease and aspartate transcarbonylase.

Prof. M. JULIA (École Normale Supérieure, Paris) dealt with mechanistic studies on free radical cyclizations. Special attention was given to the 4-phenylbutyl radical and analogues carrying naphthyl- and vinyl-groups instead of phenyl. By careful analysis, including isotopic labelling, complex cyclization pathways were unravelled.

Dr. R. SUSTMANN (University of Munster) showed that very short-lived radicals or ionic species are possible along the reaction pathway taken in cycloadditions. His interest was focussed on Diels Alder reactions and 1,3-

dipolar addition, both allowed according to the Woodward-Hoffmann formalism. The influence of substituents in each reaction component on velocity and regiospecificity was predicted with a simple perturbational treatment involving interaction of the HOMO of one reaction partner and the LUMO of the other (and *vice versa*).

The influence of substituents also played a dominant role in the lecture of Prof. S. TRIPPETT (University of Leicester) in determining the stereochemistry of phosphorus compounds. Substitutions at tetrahedral phosphorus proceed through a pentavalent bipyramidal intermediate, in which substituents can migrate between apical and equatorial positions. Migratory aptitudes of substituents depend on apicophilicity, bulk and ring strain (in the case of interconnected ligands).

Prof. R. BRESLOW (Columbia University, New York) applied electrochemistry to physical organic problems, by considering carbenium ions, radicals, and carbanions, as different oxidation states of trivalent carbon. Electrochemical correlation leads to a fascinating new approach in determining the thermodynamic properties of highly unstable species, such as the cyclopropenyl anion, cyclopentadienyl cation, and cyclobutadienes. The nonideal behaviour of some redox processes is caused by rapid secondary reactions of the generated species, but this does not affect the results seriously.

Very unstable species were also encountered in the work described by Prof. O. L. CHAPMAN (Iowa State University), resulting from exciting photochemistry at 8 K in an argon-matrix. Primary photoproducts, such as benzyne pentalene and cyclobutadiene, are remarkably stable at such low temperatures and can be studied by ESR and IR, with all the advantages of improved resolution. Carefully controlled raising of the temperature reveals in great detail the thermal behaviour of several intriguing photoproducts, which kept the audience spellbound to the very end.

The Conference was officially closed by Prof. H. ZOLLINGER, member of the Advisory Board and initiator of the series of IUPAC Conferences on Physical Organic Chemistry. It was announced that the next Conference will be held in Montpellier in September 1976.

J. W. VERHOEVEN

IV INTERNATIONAL CONFERENCE ON NONAQUEOUS SOLUTIONS

Vienna, 10-12 July 1974

The Conference was held at the Technical University of Vienna. It was organized by Verein Österreichischer Chemiker with the sponsorship of IUPAC and the Ministry of Science and Research of the Austrian Federal Government. IUPAC was officially represented by Prof. A. SWINARSKI (Torún) of its Division of Inorganic Chemistry.

Scientists from 24 countries attended, coming from as far afield as Australia, Japan, and India. Rather large delegations were present from Austria, Canada, Federal German Republic, France, Hungary, Italy, Poland, Romania, Switzerland, UK, and USA. The other countries represented were Belgium, Czechoslovakia, German Democratic Republic, Israel, Libya, Lebanon, Netherlands, Portugal, Sweden, and Yugoslavia. The total attendance was 210, 178 of whom were from countries other than Austria.

Five plenary lectures (to be published in *Pure and Applied Chemistry*, provisionally Vol. 41, No. 3, 1975) and 92 papers were presented. The first plenary speaker, Prof. A. I. POPOV (Michigan State University), discussed the application of far and mid IR, Raman, and alkali metal NMR techniques to the study of nonaqueous solutions. He showed that sodium-23 chemical shifts in different solvents show a linear relationship with Gutmann's donor numbers (donicities) for these solvents. Dr. U. MAYER (Technical University of Vienna) gave conclusive evidence for the limitations and shortcomings of the application of elementary electrostatic considerations to nonaqueous solvents. He showed the usefulness of the application of the donicity concept to molecular complexes, ionization and ion association phenomena, the electrochemical reduction of metal ions, and the kinetics of substitution reactions. Prof. H. HOFFMANN (University of Erlangen) showed the relationship between solvent donicity and substitution rates. Dr. D. H. KERRIDGE (University of Southampton) discussed the applicability of fused salt media for the preparation of various types of chemical compound. Prof. J. B. SENIOR (University of Saskatchewan) described reactions in strongly acidic media and demonstrated their usefulness for the formation of polycationic species.

The main conclusions to be drawn were as follows:

1. Modern physical methods are extremely valuable tools for the elucidation of solution structures, including those of solvent mixtures.
2. Empirical parameters, such as solvent donicity, are considerably more useful than elementary electrostatic solvent parameters.
3. The role of the outer-sphere effects in solution chemistry has been emphasized.

The Conference was characterized by the atmosphere of harmony. Verein Österreichischer Chemiker gave a reception in the Main Chemical Library of the Technical University of Vienna.

V. GUTMANN

FORTHCOMING IUPAC-SPONSORED SYMPOSIA

II INTERNATIONAL CONGRESS ON INDUSTRIAL WASTE WATER AND WASTES

Stockholm, 4-7 February 1975

The Ist International Congress on Industrial Waste Water was held in Stockholm on 2-6 November 1970. The programme attracted more than 700 participants from over 30 nations. The emphasis of the Ist Congress was on internal measures to abate water pollution in industry [proceedings published in *Pure Appl. Chem.* **29** (1-3), (1972); also available from Butterworths (London) as a hard-bound book at \$33.00/£11.00].

The programme for the IInd International Congress on Industrial Waste Water and Wastes aims at summarizing recent developments within this field and especially questions on in-plant waste water control, treatment, recycling, reuse and disposal of industrial waste water and other industrial wastes, solid as well as liquid. Special attention will be given to problems that arise in the following industries:

Chemical Industries (inorganic and organic)

Metal and Metal Processing Industries (iron and steel, and nonferrous)

Food Industries (food preservation and fermentation)

Pulp and Paper Industries (chemical pulping, paper, fibre building board)

There will also be plenary sessions on Monitoring and Control of Effluents and on Relation of Treatment and Ecological Effects. For the main lectures 14 prominent experts have been specially invited: their papers will be published in *Pure and Applied Chemistry*. In addition, discussion papers submitted by Congress participants will be presented and discussed. These will be published in the IAWPR series *Progress in Water Technology*, at the discretion of the Executive Editor.

The IInd International Congress directs itself essentially to all participants from industry concerned with industrial environmental problems. It will be sponsored by IUPAC and cosponsored by IAWPR.

General Information

The site of the Congress will be the Old Parliament House in Stockholm. The official language will be English: simultaneous translation will not be arranged. Arrangements for hotel accommodation are available through the Organizing Committee. A social programme, including a banquet, is being arranged. A number of study tours to Swedish industries with interesting solutions to waste water and waste problems will be organized during the Congress.

Further information is available from the Congress Secretariat at:

II International Congress on Industrial
Waste Water and Wastes
POB 5607, S-114 86 Stockholm 5
Sweden

Telephone: 08 222540

Telegrams: Wastecongress Stockholm

IV BRATISLAVA INTERNATIONAL CONFERENCE — MODIFIED POLYMERS, PREPARATION AND PROPERTIES

Bratislava, 1-4 July 1975

This Conference is being organized under the sponsorship of IUPAC by the Polymer Institute of the Slovak Academy of Sciences, in cooperation with the Macromolecular Division of the Slovak Chemical Society and with the Department of Chemical Technology of Plastics and Fibres of the Slovak Technical University.

Scientific Programme

The scientific programme of the Conference will encompass the following fields:

Chemical and physical processes of modification of the molecular and supermolecular structure of preformed polymers

Properties of modified polymers in both the solid state and solution

About 8 main lectures are intended to be presented, and these will be published in the official journal of IUPAC, *Pure and Applied Chemistry*.^{*} The Organizing Committee is pleased to invite the presentation of short communications on the above topics. Contributed papers may be presented in any language, but the Organizers suggest that speakers should preferably use English. Simultaneous translation will not be arranged.

Correspondence

Further information about the scientific programme, Conference fees, instructions for preparation and publication of manuscripts, final registration forms and accommodation facilities, social events, *etc.*, may be obtained by writing to the Chairman of the Organizing Committee:

Dr. A. ROMANOV
Polymer Institute
Slovak Academy of Sciences
Dúbravská Cesta
CS-809 34 Bratislava
Czechoslovakia

25th IUPAC CONGRESS

Jerusalem, 6-11 July 1975

The Congress will take place at the campus of the Hebrew University in Western Jerusalem. The scientific programme will consist of some 40 invited lectures and a large number of contributed papers, in four divisions:

- A. Organic Chemistry
- B. Physical Chemistry
- C. Medicinal Chemistry
- D. Applied Chemistry

^{*}The plenary and main lectures from the previous meeting in this series, 'Chemical Transformations of Polymers', were published in *Pure Appl. Chem.* **30**(1-2), (1972) and also issued as a hard-bound book by Butterworths (London) at \$25.50/£8.50.

The plenary lectures will be published by IUPAC. A booklet containing the abstracts of the contributed papers will be distributed to the participants at the Congress. The full papers may be published anywhere by the authors after the Congress. The official language is English. Papers may be presented in any language, but the use of one widely understood is recommended. The Organizing Committee regrets that it cannot provide simultaneous translation.

Division A: Organic Chemistry

Plenary Lectures

- H. C. BROWN (Lafayette, USA): Organoboranes—the modern miracle
E. HAVINGA (Leyden, Netherlands): New results in the photochemistry of aromatic compounds

Sections/Main Section Lectures

1. New theoretical insights into organic molecules
K. FUKUI (Kyoto, Japan)
2. Chemistry of excited states
K. SCHAFFNER (Geneva, Switzerland)
3. Novel instrumental methods of structure determination
C. DJERASSI (Stanford, USA)
4. Computers in organic synthesis and structure determination
W. T. WIPKE (Princeton, USA)
5. Novel synthetic applications of organometallic compounds
To be announced
6. Ylid Chemistry
G. WITTIG (Heidelberg, Federal Republic of Germany)
7. Prebiotic chemistry and organic geochemistry
L. E. ORGEL (La Jolla, USA)
8. Approaches to the structure of biological receptors
J. P. CHANGEUX (Paris, France)—held jointly with the Division of Medicinal Chemistry
9. Stereochemical aspects of biogenesis
D. LAVIE (Rehovot, Israel)

Division B: Physical Chemistry

Plenary Lectures

- D. HERSCHBACH (Cambridge, USA): Molecular dynamics of chemical reactions and collisional energy transfer
E. B. WILSON (Cambridge, USA): 50 years of quantum chemistry

Section/Main Section Lecturers

1. Condensed phases
F. H. STILLINGER (Murray Hill, USA)
2. Lasers in chemistry
C. B. MOORE (Berkeley, USA)
3. Molecular spectroscopy
I. ROSS (Canberra, Australia)
4. Molecular dynamics
J. T. LEE (Chicago, USA) and
R. BERSOHN (New York, USA)

5. Interfacial electrochemistry
H. GERISCHER (Berlin, Federal Republic of Germany)
6. Molecular structure
D. A. SHIRLEY (Berkeley, USA)
7. Molecular conformations
P. G. DE GENNES (Orsay, France)
8. Symposium: 50 years of quantum chemistry
The speakers—in addition to the plenary lecturer—to be announced

Division C: Medicinal Chemistry

Plenary Lecture

S. SPIEGELMAN (New York, USA): A molecular approach to the etiology of human cancer

Section/Main Section Lecturers

1. Intermediate products in drug metabolism as a basis of drug action and toxicity
To be announced
2. Compounds modulating biosynthesis and degradation of prostaglandins
B. SAMUELSON (Stockholm, Sweden)
3. Chemotherapy of tropical diseases
To be announced
4. Chemistry and biochemistry of ageing
To be announced
5. Symposium: Chemistry of memory
The panel of speakers includes
S. P. R. ROSE (Bletchley, UK)
G. UNGAR (Houston, USA)
S. H. BARONDES (San Diego, USA)
H. HYDEN (Göteborg, Sweden)
6. Immunosuppression
To be announced
7. Approaches to the structure of biological receptors
J. P. CHANGEUX (Paris, France)—held jointly with the Division of Organic Chemistry

Division D: Applied Chemistry

Plenary Lecture

G. WILKE (Mülheim, Federal Republic of Germany): Homogeneous transition metal catalysts in applied chemistry

Section/Main Section Lecturers

1. New techniques in chemical processing
 - (a) Ion exchange, solvent extraction
A. BANIEL (Haifa, Israel)
 - (b) Microbiological methods
J. V. BECK (Provo, USA)
2. Symposium: Chemical aspects of future energy sources
The panel of speakers will be announced

3. Food resources through chemistry
To be announced
4. Surface chemistry and surface activity
 - (a) Solid-liquid surfaces in aqueous solutions
D. H. EVERETT (Bristol, UK)
 - (b) High temperature solid-gas reactions
To be announced
5. Chemical processes for water desalination
S. LOEB (Beer Sheva, Israel)
6. Recycling and reuse of wastes
 - (a) Waste banks as a solution to industrial waste problems
H. O. BOUVENG (Stockholm, Sweden)
 - (b) Reuse and disposal of waste acids
G. THEILIG (Frankfurt, Federal Republic of Germany)

Intending participants are invited to submit papers in the various sections enumerated in the scientific programme. The Scientific Committees of the four Divisions will meet in February 1975 and select those papers which can be presented at the Congress. The deadline for receipt of abstracts for consideration by the Scientific Committees is 75.2.1. No guarantee can be given that an abstract received later will be considered for inclusion in the programme.

Abstracts must be submitted as the original typescript plus two carbon copies on good white paper of format 12x18 cm. The abstract should be typed *single-spaced*, and should not exceed 25 lines. The entire TITLE should be capitalized, followed by the name(s) of the author(s) (the name of the author presenting the paper *underlined*) and the institution. Start abstract on a new line, and indent all paragraphs. Formulae and special symbols should be drawn in black ink.

Only slides of standard 5 x 5 cm size (35-mm film) can be projected. They should be easily legible from a distance of 20 m in a darkened room. Positive black on white slides are preferable. Tables with data should be avoided.

Registration

Further information on the Congress and details of registration may be obtained from:

Organizing Committee
25th IUPAC Congress
POB 983, Jerusalem
Israel

INTERNATIONAL SYMPOSIUM ON MACROMOLECULES

Jerusalem, 13-18 July 1975

The Symposium, which will constitute the III Aharon Katzir-Katchalsky Conference is being organized under the auspices of IUPAC, the Israel Academy of Sciences and Humanities, and the Israel Chemical Society, by the Aharon Katzir-Katchalsky Center of the Weizmann Institute of Science.

Tentative Scientific Programme

The Symposium will be divided into nine sections. Both plenary and sectional lectures are being planned.

1. *Polymer Theory*
(with special emphasis on the solid state and on computer simulation)
2. *Surface and Electrochemistry of Macromolecules*
(structure of polymers and macromolecules at interfaces, with special emphasis on the surface charge effect in polymer interactions)
3. *Ions and Polar Molecules in Polymeric Solids*
(small ions as probes for the dynamics of solid polymeric matrices; ionic conductivity in amorphous solid polymers; solid polymers as host materials for photosensitive and photoactive ions and small molecules—recording and electrooptical materials)
4. *Polymers as Chemical Reagents*
(use of polymers as reagents and carriers in general organic synthesis, e.g., polymer attached catalysts, polymeric transfer agents, polymeric carriers, polymers as immobilizing media)
5. *Artificial Membranes—Synthesis and Function*
(transport and structural properties of synthetic membranes; relation between membrane structure and mechanism of permeation; specific and nonspecific permeation of gases, solutes, and solvents; theoretical considerations and practical application of membranes in desalination and industrial separation processes)
6. *Polymers in Pollution Abatement*
(utilization of polymeric membranes; special resins and polymeric additives in water purification; accelerated degradation of synthetic polymeric materials)
7. *Biomedical Applications of Macromolecules*
(substitute synthetic materials, compatibility with biological tissue; use in bioengineering; use in pharmacology; biostability and biodegradability)
8. *Specialized Polymers in High Performance Composites for Structural Application*
(high performance polymeric fibres and matrices for engineering structural applications (aerospace, etc.); matrix-filler interactions)
9. *Structure and Properties of Natural Fibre Forming Polymers*
(formation and origin of structure of natural fibre forming polymers (polysaccharides, keratin, collagen, etc.); properties as related to structure; chemical and physicochemical modifications imparting new emphasis on flame resistance and thermal stability)

Free Communications on the nine topics listed will be considered. The presentation of a paper plus time for discussion will be 15 minutes. Those intending to submit a paper are asked to indicate a provisional title. It is expected that participation will have to be limited to the presentation of one paper only. Extended abstracts of between 500-1000 words must be submitted by 75.2.1. The Symposium will be conducted in English, but papers may be presented in any widely understood language. The use of English is, however, recommended because no facilities for simultaneous translation can be provided.

Travel and Accommodation

Peltours Ltd. (Congress Department: 52 Nachlat Benyamin St., Tel Aviv, Israel; telephone: 50851; telex: 03-3803; telegrams: PELTOURS TEL AVIV) has been appointed the official travel agent and will provide all necessary services to participants. Its offices and agents abroad will aim to offer the best possible travel arrangements to and from Israel. Both from USA and Europe there are specially reduced prices for group travel and in some cases also for individual inclusive tours. It should be noted that members of existing organizations may under certain conditions take advantage of special affinity group travel arrangements which are lower than the regular group travel rates. In Israel, Peltours, through its head office and branches throughout the country, will be responsible for hotel accommodation, meet participants on arrival, arrange transfer to hotels, and provide sightseeing programmes. Hotel accommodation has been reserved in hotels of all grades (5-star, 4-star, and 3-star, with a limited number of rooms available in low price hotels).

The weather in Jerusalem in July is uniformly sunny during the day and cool in the evenings.

Secretariat

All enquiries concerned with the meeting should be addressed to the Secretariat at:

IUPAC Symposium on Macromolecules
Aharon Katzir-Katchalsky Center
Weizmann Institute of Science
POB 16271, Tel Aviv
Israel

IX INTERNATIONAL CONGRESS OF CLINICAL CHEMISTRY

Toronto, 13-18 July 1975

The Congress will offer special opportunities for contact with new scientific and technical advances in clinical chemistry, as well as the chance of exciting vacation travel in Canada and USA. It will be held in the Four Seasons-Sheraton Hotel, Toronto, a new hotel specially designed for largescale conferences. All the principle scientific presentations will be held in very well equipped lecture theatres of the hotel complex, which will also house the trade exhibition. The hotel is situated in the centre of the Down-Town area, immediately adjacent to the City Hall, and has restaurants, bars, and shopping facilities within the building. It is also within a few minutes walk of airline offices, numerous restaurants (many of special ethnic character), cinemas, concert halls, *etc.* Parking facilities are available at the hotel and in adjacent parking buildings.

A group of six University Teaching Hospitals is situated within a mile of the Congress building, and tours of selected departments will be arranged. A Congress travel agency will be situated in the hotel, and will attend to all pre- and post-Congress tours, many of which will be offered at favourable rates. Lisind International Canada Ltd. (335 Bay Street, Suite 704, Toronto, Ontario M5H 2R3, Canada; telephone: 868 0845) has been appointed as the official travel bureau. Lisind International in cooperation with CP Air and KLM Royal Dutch Airlines can offer special group tours and individual

travel from many countries to Toronto. For all Registrants, a full programme of social events and local tours, including lakefront outings, will add to the enjoyment of the Congress week.

Scientific Programme

The IX Congress is organized by the Canadian Society of Clinical Chemists and the American Association of Clinical Chemists on behalf of IFCC and IUPAC. There will be plenary sessions, symposia, and scientific papers, both invited and contributed. The official working language of the Congress will be English.

Symposia will cover the following subjects:

- Clinical Chemistry in Pediatrics
- Mechanisms of Hormone Action
- New Concepts of Interpretation of Laboratory Data
- Biochemical Aspects of Hyperalimentation
- Metabolic Regulation
- Clinical Chemistry—Perspectives of a Changing Discipline
- Emerging High Sensitivity Analytical Techniques
- Clinical Significance of Measurement of Drug Levels in Body Fluids
- Immunology—Interrelations with Clinical Chemistry
- Referee Methods—Current Status and Significance for Patient Care
- Diagnostic Biochemistry and Tissue Culture

Secretariat

For further information, please write to the following address:

IX International Congress of Clinical Chemistry
Toronto Dominion Centre
POB 34, Toronto
Ontario MK5 1B7
Canada

***IV INTERNATIONAL SYMPOSIUM ON CAROTENOIDS**

Berne, 25-29 August 1975

The Symposium will be sponsored by IUPAC and the Swiss Science Council, Comité Suisse de Chimie, and the Swiss Chemical Society. The tentative scientific programme includes session lectures and contributed papers on recent progress in the field of carotenoids. The following sessions are planned:

- Physical Methods
- Complexed Carotenoids
- Structures, Stereochemistry, Syntheses, Reactions
- Technology
- Abscisic Acid and Related Compounds
- Biochemistry

The 10-12 session lectures (to be published in *Pure and Applied Chemistry*) will be followed by contributed papers with the exception of the session on

*The plenary lectures from the III Symposium were published in *Pure Appl. Chem.* 35(1), (1973) and also issued as a hard-bound book by Butterworths (London) at \$11.40 £3.80.

Technology, when the participants will be invited to take part in the official excursion. A programme for the ladies is in preparation.

Correspondence

Correspondence should be addressed to:

Dr. H. PFANDER, Secretary General
IV International Symposium on Carotenoids
University Institute of Organic Chemistry
Länggass-Strasse 7, CH-3012 Berne
Switzerland

INTERNATIONAL ROUND TABLE ON STUDY AND APPLICATIONS OF TRANSPORT PHENOMENA IN THERMAL PLASMAS

Font Romeu, 12-16 September 1975

The Round Table is being organized by the Sub-Commission on Plasma Chemistry of IUPAC at Laboratoire des Ultra-Réfractaires du CNRS at Odeillo, Font Romeu (France). Technical sessions are planned on the following topics:

I. Largescale Plasma Heating

Application to inert and reactive gases heating

Organizer and Animator: Mr. J. FABRE (2 Rue Louis Murat, F-75008 Paris, France)

Invited Speaker: Dr. P. H. WILKS (IONARC, USA)

II. Heat Transfer to Condensed Phases

Application to technology of plasma furnaces; to melting, spheroidization of refractory materials; to chemical reactions (without mass transfer from or to the plasma)

Organizer and Animator: Dr. J. LAWTON (Electricity Council Research Centre, Capenhurst, Chester CH1 6ES, UK)

Invited Speaker: Prof. E. PFENDER (University of Minnesota, USA)

III. Simultaneous Heat and Mass Transfer

Application to evaporation and condensation of refractory materials; to chemical reactions; to preparation of layers from vapour phase

Organizer and Animator: Dr. W. H. GAUVIN (Noranda Research Centre, 240 Boulevard Hymus, Pointe Claire 730, Québec, Canada)

Invited Speaker: Dr. I. G. SAYCE (National Physical Laboratory, UK)

IV. Simultaneous Heat and Momentum Transfer

Application to sedimentation, fluidization; to plasma spraying

Anyone wishing to present a contribution is invited to write to the appropriate session Animator (or for Session IV to Dr. C. BONET, Laboratoire des Ultra-Réfractaires du CNRS, BP 5, Odeillo, F-66120 Font Romeu, France), enclosing a brief summary (50-100 words) of the proposed contribution. Contributions may be offered in any language, although it is hoped that speakers will use a language that is commonly understood by most participants. The closing date for receipt of abstracts is 75.3.1.

Anyone requiring further details should write to the Chairman of the Organizing Committee:

Prof. M. FOEX
Laboratoire des Ultra-Réfractaires du CNRS
BP 5, Odeillo, F-66120 Font Romeu, France

**INTERNATIONAL CONFERENCE ON
COLLOID AND SURFACE SCIENCE
Budapest, 15-20 September 1975**

The Conference is being organized by the Hungarian Chemical Society jointly with the Commission of Colloid Chemistry of the Hungarian Academy of Sciences, under the sponsorship of IUPAC. The programme will cover all aspects of colloid and surface science, including surface and colloid chemistry of macromolecular systems. Main lectures will be presented by invitation only. Short communications (20 minutes each with discussion) will be accepted in limited number.

The working language will be English. Although papers (except main lectures) can be presented in any widely understood language, the use of English is recommended, because no translation facilities will be provided. Main lectures will be published in *Pure and Applied Chemistry*, the official journal of IUPAC, and also made available as a specially bound reprint. Extended abstracts of contributed papers will be available for participants before the Conference.

Correspondence

All correspondence concerning the Conference should be addressed to:

Prof. E. WOLFRAM, Secretary
International Conference on Colloid and Surface Science
Department of Colloid Science
Loránd Eötvös University
Puskin u. 11-13
H-1088 Budapest
Hungary

**VI INTERNATIONAL CONGRESS ON CATALYSIS
London, 12-16 July 1976**

It is intended that the Congress, which will be held at Imperial College of Science and Technology, will be concerned with a number of themes in the general field of heterogeneous catalysis and with some related aspects of chemical engineering and of homogeneous catalysis. Topics 1-4 will be the major themes of the Congress and it is expected that more time will be devoted to these than to topics 5-10.

1. *Catalytic activity and surface topography*
To include chemical bonding and surface coordination, particle size, and the effects of atoms neighbouring the active site.
2. *Catalyst preparation and characterization*
To include decay, ageing and regeneration, and interaction of catalyst components.
3. *Modelling of catalytic reactions*
To include transport processes, optimization, stability of catalysts, and new experimental reactor configurations.
4. *Surface composition of reacting systems*
To include new techniques and theoretical calculations to reveal the nature of intermediates and excited states.
5. *Organic and metalloorganic catalysts*
To include immobilized enzymes and supported complexes.

6. *Two-component systems as selective catalysts*
To include alloys, binary oxides, etc., and related supported catalysts.
7. *Electrocatalysis*
To include fuel cell electrodes.
8. *Asymmetric catalysis and stereospecific catalysis*
To include hydrogenation and polymerization.
9. *Hydrocracking, hydroforming, and hydrode-sulfurization*
To include pure and applied aspects.
10. *Applications of catalysis to problems of current industrial importance*

Scientific Programme

The programme will consist of 5 plenary lectures and 100 contributed papers. If more papers are offered than can be accommodated in the programme, those papers will be selected which, in the judgement of the Committee, make the most significant contributions to the themes of the Congress. Initial selection will be on the basis of abstracts of 500 words, which should be received no later than 75.5.1. Authors will be advised whether or not they should subsequently submit a full paper. The last date for receipt of full papers will be 75.9.20. It is planned to arrange the programme on the basis of two parallel sessions.

The official language of the Congress will be English. Arrangements for translation will not be made and thus papers, abstracts, and presentation, should be in English. It is intended to provide time for adequate discussion of the contributed papers. The presentation of the papers will necessarily be limited to an abbreviated form and the discussion will be as informal as possible. The papers will be preprinted in full and distributed to all participants in advance of the Congress. The entire proceedings will be published and will be available to participants at a reduced price.

Accommodation

The scientific sessions will take place in lecture theatres at Imperial College. Accommodation will be available in modern halls of residence situated adjacent to the College. Hotels in the area of the Congress are plentiful, but in view of the meeting taking place during the tourist season, participants wishing to stay in hotels are advised to secure reservations in good time.

Imperial College is situated close to central London and all the facilities of the city are within easy reach. A programme of evening social events is planned for the week of the Congress, and on Wednesday afternoon no scientific session will be held so that participants may arrange their own meetings or other activities. Special events are being planned for the ladies, including sightseeing excursions as well as shopping tours and visits to buildings of interest in and around London.

Correspondence

All correspondence concerning the Congress should be addressed to:

Dr. JOHN F. GIBSON
VI International Congress on Catalysis
Chemical Society
Burlington House, Piccadilly
London W1V 0BN
UK

ASSOCIATED ORGANIZATIONS OF IUPAC

II EUROPEAN CONFERENCE ON ANALYTICAL CHEMISTRY

Budapest, 25-30 August 1975

The Working Party on Analytical Chemistry of FECS is organizing 'Euro-analysis II' at the Technical University of Budapest. There will be 10 invited lecturers (45 minutes each with 10 additional minutes for discussion) by leading authorities in the following fields:

Optimization of Analysis

Voltammetric Analysis

Flame Photometry, Atomic Absorption and Atomic Fluorescence Spectroscopy

Selective Ion-Sensitive Electrodes

Instrumental Methods for Organic Analysis

What Can We Really Do with Computers in Analytical Chemistry?

Liquid Chromatography

Thermal Analysis

Environmental Analysis

Role of Analytical Chemistry in Research of Metabolisms

In addition, there will be original unpublished papers covering all aspects of analytical chemistry. The Organizing Committee prefers English as the working language for presentation and discussion of papers. No translation services will be provided. All Conference materials will be published in English.

All correspondence should be addressed to:

EUROANALYSIS II

c/o Hungarian Chemical Society

POB 240, H-1368 Budapest

Hungary

Telephone: 427343

Telegram: Kémikusok—Budapest

VII INTERNATIONAL CONGRESS ON RHEOLOGY

Göteborg, 23-27 August 1976

The Congress is being organized at Chalmers University of Technology by the Swedish Rheological Society, a special section of the Swedish National Committee on Mechanics, under the auspices of the International Committee on Rheology.

Further information will be available shortly from the Chairman of the Organizing Committee:

Prof. J. KUBÁT

Chalmers University of Technology

Fack

S-402 20 Göteborg

Sweden

ACTIVITIES OF OTHER INTERNATIONAL UNIONS

INTERNATIONAL CONFERENCE ON IMPROVEMENT OF PHYSICS EDUCATION

Edinburgh, 29 July-6 August 1975

This Conference will be held under the sponsorship of IUPAP, in association with UNESCO, at the University of Edinburgh. The principal objectives will be:

- (i) to identify and analyze the present problems and recent trends in physics education at all levels, with particular reference to secondary school and undergraduate university courses;
- (ii) in the light of this analysis, to prepare guidelines for plans of action—involving international, regional, and national organizations—for the further improvement of physics education.

Anyone who wishes further information should write to the Secretary of the Local Organizing Committee, Dr. R. M. SILLITTO, Department of Physics, University of Edinburgh, Mayfield Road, Edinburgh, UK.

GENERAL ASSEMBLY AND INTERNATIONAL CONGRESS OF CRYSTALLOGRAPHY

By invitation of the Fundamenteel Onderzoek der Materie met Röntgen en Elektronenstralen (FOMRE), the X General Assembly and International Congress of Crystallography will be held in Amsterdam, during 7-15 August 1975.

The arrangement of the scientific programme will, in general, be similar to that of the IX Congress held in Japan in 1972. There will be general lectures, scientific sessions on topics of interest for today's crystallography and chemistry, poster sessions, open sessions of Commissions of IUCr, and *ad hoc* meetings.

Participants are invited to submit abstracts of recent work on crystallographic subjects. Upon acceptance, these contributions will be printed in the book of abstracts of the Congress. For oral presentation in the formal scientific sessions or for the poster sessions, a selection will be made from the papers lying within the range of the Congress topics. The *ad hoc* meetings are intended mainly to encourage free discussion.

A commercial exhibition will be organized in which manufacturers and distributors of equipment related to crystallographic research may display their products. Further information can be obtained from the Organizing Committee. For the accompanying members, a choice of tours will be offered.

The Congress Organizing Committee consists of Prof. D. FEIL (Chairman), Dr. P. B. BRAUN (Vice-Chairman), Dr. H. M. RIETVELD (Secretary and Treasurer), Mrs. R. OLTHOF, Prof. G. D. RIECK, and Dr. H. SCHENK. Correspondence should be addressed to: The Organizing Committee, X International Congress of Crystallography, POB 7205, Amsterdam, Netherlands. Telephone: (020) 440807; telegram: ORBU Amsterdam; telex: 13499 (RAICO).

XVI GENERAL ASSEMBLY OF IUGG

Grenoble, 25 August-6 September 1975

The object of the International Scientific Unions is to promote and coordinate scientific research activities between their different adhering national bodies. During the General Assemblies of the Unions, programmes of international cooperation are studied, and those which are expected to be of major importance for the development of science are adopted. In addition to such planning activity, the scientists taking part in a General Assembly compare the results of their studies and exchange their ideas during the course of the symposia, and in informal discussion groups. This double activity is particularly important in fields covered by the International Union of Geodesy and Geophysics, which since 1963, meets in General Assembly only every 4 years. A number of specialized symposia are held between Assemblies but the results of the studies in the seven disciplines represented in IUGG are all brought together only on the occasion of these four-yearly Assemblies. That is why participation in these meetings is steadily increasing and considered to be very important because of the rapid rate of development in geophysical sciences.

Programme

The official opening will be held on 25 August at 10 a.m. at the Palais de Glace, a beautiful building which was finished for the 1968 Winter Olympic Games. During the preceding week some of the Associations will hold administrative and Commissions meetings. During the General Assembly a programme of 33 symposia is being organized, the list of which is given below. These symposia will be held on the University campus of Saint-Martin d'Hères.

1. *Role of Geophysics, Geochemistry, and Experimental Petrology in the Division of Earth Models*
Conveners: P. J. WYLLIE, University of Chicago, Department of Geophysical Science, 5734 South Ellis Avenue, Chicago, Illinois 60637.
R. O'CONNELL, Department of Geological Science, Harvard University, Cambridge, Massachusetts.
2. *Theory and Experiment Relevant to Geodynamic Processes*
Convener: O. ANDERSON, UCLA, Institute of Geophysics and Planetary Physics, Los Angeles, California 90024.
3. *Heat Flow and Geodynamics*
Convener: E. LUBIMOVA, Geophysical Committee, Molodezhnaya 3, Moscow B-296.
4. *Geophysical Phenomena Preceding, Accompanying, and Following Earthquakes*
Convener: A. ZATOPEK, Institute of Geophysics, Charles University, Ke Karlovu, Praha 2.
5. *Recent Crustal Movements*
Convener: P. VYSKOCIL, Research Institute for Geodesy, Nadrezní 31, Praha 5 Smichov.
6. *Magnetic Properties of Basalts and their Relation to Magnetic Anomalies*
Convener: Not yet known.

7. *Secular Changes of Magnetic Anomalies and their Relation to Stress Patterns*
Convener: Not yet known.
8. *Planetary Atmosphere Evolution*
Convener: Not yet known.
9. *Analysis, Processing, and Interpretation of Geophysical Data*
Convener: Not yet known.
10. *Mid-Ocean Ridges, Oceanic Trenches, and Geodynamics*
Convener: S. UYEDA, Earthquake Research Institute, University of Tokyo, Bunkyo-ku, Tokyo 113.
11. *Ancient Plate Margins*
Convener: Not yet known.
12. *Submarine Volcanism*
Convener: Not yet known.
13. *Deep Sea Drilling: the History of the Ocean*
Convener: N. T. EDGAR, Scripps Institution of Oceanography, University of California, POB 109, La Jolla, California 92037.
14. *Deep Structure of Volcanoes*
Convener: D. SHIMOZURU, Earthquake Research Institute, University of Tokyo, Bunkyo-ku, Tokyo 113.
15. *Largescale Modification of Fresh Water Systems and their Effects on Oceanic Environment*
Convener: J. A. ELLIOTT, Atlantic Oceanographic Institute, Bedford Institute of Oceanography, Dartmouth, Nova Scotia B2Y 4A2.
16. *Meteorological and Hydrological Aspects of Continental Droughts*
Convener: Not yet known.
17. *Isotopes and Impurities in Snow and Ice*
Convener: Not yet known.
18. *GARP First Objective: Weather Predictability*
Convener: Not yet known.
19. *GARP Second Objective: Climatic Change*
Convener: Not yet known.
20. *Marine Pollution*
Convener: M. UDA, 8-5-9 Okuzawa, 8-Chome, Setagaya-ku, Tokyo 158.
21. *Atmospheric Pollution*
Convener: Not yet known.
22. *Stratosphere-Mesosphere Relations*
Convener: Not yet known.
23. *Optical Sensing and Probing of the Atmosphere*
Convener: Not yet known.
24. *Tidal Interactions (including Earth Tides)*
Convener: O. SCHNEIDER, Osservatorio Astronomico, Paseo del Basque, La Plata.
25. *Global Effects of the Interplanetary Medium—Magnetosphere—Lower Atmosphere Interactions*
Convener: Not yet known.

26. *Physical Chemistry and Inorganic Chemistry of Sea Water*
Convener: J. M. GIESKES, Scripps Institution of Oceanography,
 University of California, POB 109, La Jolla, California 92037.
27. *Geochemistry of the Sea*
Convener: H. CRAIG, Geological Research Division, Scripps Institu-
 tion of Oceanography, University of California, POB 109, La Jolla,
 California 92037.
28. *Motion and Structure of Oceans under a Time-Dependent Atmosphere*
Convener: E. C. LAFOND, Naval Undersea Center, San Diego,
 California 92132.
29. *Marine Geodesy (including Mean Sea Level)*
Convener: G. MOURAD, Battelle Memorial Institute, Columbus
 Laboratories, 505 King Avenue, Columbus, Ohio 43201.
30. *Ocean Optics*
Convener: N. JERLOV, Institute of Physical Oceanography, University
 of Copenhagen, Haraldsgade 6, Copenhagen N.
31. *High Atmosphere and Space Problems in Atmospheric Electricity*
Convener: Not yet known.
32. *Artificial Weather Modification*
Convener: Not yet known.
33. *Thermal and Chemical Problems of Thermal Water*
Convener: Not yet known.

For further information, please write to:

Comité National Français de Géodésie et Géophysique
 136 bis, Rue de Grenelle
 F-75700 Paris
 France
 Telephone: 555 4345

II WORLD CONFERENCE ON COMPUTERS IN EDUCATION

Marseille, 1-5 September 1975

This multidisciplinary Conference will be held under the sponsorship of the International Federation for Information Processing, with cosponsorship by other organizations including the IUPAP Commission on Physics Education. The Conference aims to bring together people concerned with the many possible roles of informatics in education. At an earlier Conference on the subject it was concluded that a distinction must be made between the methodology of informatics and the computer, and that there were considerable advantages to be gained by introducing the methodology of informatics into the teaching of all disciplines. The 1975 Conference will show progress made in this direction and attempt to gain new insight for the future.

A call for papers has been issued. For detailed information, please write to the Chairman of the Programme Committee, Mr. J. HEBENSTREIT, École Supérieure d'Électricité, 10 Avenue Pierre-Larousse, F-92240 Malakoff, France.

INTERNATIONAL CONFERENCE ON TEACHING PHYSICS FOR RELATED SCIENCES AND PROFESSIONS

Seattle, probably Summer, 1976

The Conference now being planned will be held under the sponsorship of the IUPAP Commission on Physics Education on the campus of the University of Washington. It will deal with the teaching of physics to students in related scientific and professional fields (engineering, life sciences, chemistry, earth sciences, *etc.*) at the undergraduate university level. The Conference will bring together two categories of participant: instructors and leading professionals from fields relying on a background in physics and physics instructors who have a special concern or responsibility for courses taken by students seeking careers in other sciences and professions. Among the questions to be addressed are the following:

What is the proper role of physics in the preparation of scientists, engineers, and other technically trained persons? How much of the value of the physics background comes from exposure to an outlook on the universe derivable from a few general principles? from learning to abstract a simple model from a complex situation? from learning to apply well known laws? from learning the principles behind contemporary instrumentation? from learning to evaluate errors and uncertainties?

In contemplating the physics courses presently offered to their students, what do the related disciplines find missing? What do they find adequate?

How can physics instructors discover and devise illustrations and examples that draw upon the related disciplines and will arouse interest in the students of these disciplines?

What trends in the related disciplines have implications for physics instruction of their students and what trends in physics should influence such instruction?

Please send requests for further information to Dr. RONALD GEBALLE, Department of Physics, University of Washington, Seattle, Washington 98105, USA.

ICSU ABSTRACTING BOARD

The ICSU Abstracting Board was established in 1953 for the purposes of organizing and promoting internationally the exchange and dissemination of information by secondary processing services in science and technology, and to deal with matters related thereto.

The Board is made up of:

- 2 Representatives from ICSU
- 1 Representatives of each Member Union
- 1 Representatives of each Member Service
- 1 Representatives of each Member Country

Full Board meetings were held in July 1973 in London and in July 1974 in Berlin.

Membership of ISCU AB (as of July 1974)

In addition to the two representatives of ICSU, Prof. F. A. STAFLEU (Netherlands) and Ing. Gen. G. R. LACLAVERE (France), the Membership of the Board is now composed of:

- 4 Member Countries: Belgium, France, S. Africa*, USA
- 6 Member Unions: IAU, IUBS, IUCr, IUGS, IUPAC, IUPAP
- 20 Member Services†

The increasing size of ICSU AB has made advisable a study of its organization and committee structure. Some reorganization has been adopted for 1974 onwards.

Elections of Officers and Main Committees for 1974 onwards

The full Board meets as a General Assembly every third year and elects Officers and Main Committees for the following 3 years. 1974 is an Assembly year and the new elections were made at the July meeting in Berlin as follows:

President Dr. J. W. BARRETT

Executive Committee

Chairman: Dr. J. W. BARRETT

Vice-Chairman: Mde. N. DUSOULIER

Member Unions (3): Dr. J. W. BARRETT (IUPAC)
Prof. J. M. ZIMAN (IUPAP)
Prof. A. J. C. WILSON (IUCr)

Member Countries (2): Prof. A. BRUYLANTS (Belgium)
Dr. J. J. LLOYD (USA)

Member Services (4): Mde. N. DUSOULIER (Bulletin Signaletique)
Mr. D. B. BAKER (Chemical Abstracts Service)
Dr. C. WEISKE (Chémie Information Documentation)
Mr. D. BARLOW (INSPEC)

ICSU (1): To be appointed

Others (2): Dr. R. J. SMITH (Biological Abstracts),
Chairman of Planning and Steering Committee

Planning and Steering Committee (nominated by President)

Dr. R. J. SMITH (Biological Abstracts)—Chairman

Dr. J. W. BARRETT

Mde. N. DUSOULIER

Prof. K. FAEGRI (IUBS)

Dr. J. GRAVESTEIJN (Bibliographie des Sciences de la Terre)

Dr. A. K. KENT (UKCIS)

*S. Africa elected as new Member Country in July 1974.

†(a) CEDOCAR (Centre de Documentation de l'Armement) elected as new Member Service in July 1974.

(b) American Psychological Abstracts (APA), Japan Information Centre of Science and Technology (JICST), UK Chemical Information Service (UKCIS), and Zoological Record (ZR) elected as new Member Services in July 1973.

Dr. J. J. LLOYD (American Geological Institute)
Dr. P. V. PARKINS (Biological Abstracts)
Dr. H. VAN COTT (American Psychological Abstracts)
Prof. V. WEIDEMANN (Physikalische Berichte)

Some Major Programmes of ICSU AB

1. The draft standard for bibliographic strips, prepared under contract by the Board, has been submitted to ISO but it will be published immediately in the form of an ICSU AB-UNESCO 'guideline'.
2. An important part of the Board 'Input Plan' for the creation of a 'World System for Abstracting and Indexing Services' is to prepare an aggregate list of periodicals scrutinized by the Member Services—these number tens of thousands. The production of a base file of some 30,000 titles is being undertaken, with input from ICSU AB Member Services, by the International Centre of ISDS (International Serials Data System of UNISIST) in Paris. There has been considerable delay but it is hoped that the base file will be available by the end of the year, which will then allow an analysis of the processing of journals by Member Services, a prerequisite for any allocation of journals to specific Member Services. The overall objective is to reduce duplication and increase effectiveness of journal abstracting.
3. A common search format for computer files is desirable and a joint committee of the Board with the two associations of users of computer files in Europe and USA (EUSIDIC and ASIDIC, respectively) has agreed a programme to achieve this.
4. The ICSU AB-CODATA Joint Working Group has given consideration to the 'flagging' or 'tagging' of abstracts to indicate content of specific data. It is likely that there will be a joint programme under contract from UNESCO to produce a unified scheme. Present sporadic attempts at flagging, including two letter systems, are quite inadequate.
5. A Reference Manual has been prepared as a basis for common practices amongst Member Services. It attempts to provide an objective basis for agreement on common practices and is under examination by several major services; reception is promising.
6. ICSU AB in its July meeting agreed the enlargement and further support of the Joint Working Group on Cooperation Among Editors, which is directed towards improving and increasing cooperation between primary and secondary publication activities. Greater representation from Unions will be sought.

Activities of Subject Working Groups

There are six subject Working Groups covering Astronomy, Mathematics, Physics, Chemistry, Geology, and Biology. Their effectiveness has varied considerably with some outstanding results when a Working Group has been joint with its Union. It is likely that there will be new flexible systems developed, involving Subject Committees with maximum involvement with Unions where possible. Each Subject Committee would be empowered to set up *ad hoc* forces with defined objectives.

Relationships with UNISIST

ICSU AB was a major factor in the final creation of UNISIST within

UNESCO. A close and effective working relationship between the two organizations is necessary and is clearly developing. The Director of UNISIST, Dr. A. WYSOCKI, was present as an observer throughout the Berlin Board Meeting. An ICSU AB position paper on UNISIST has been passed to UNESCO strongly recommending that UNISIST should remain in the Science Sector.

Publications

Important general publications* during the last two years have been:

1. Survey of the activities of the ICSU Scientific Unions, special and scientific committees and commissions of ICSU in the field of scientific information during the year 1970
December 1973 200pp. \$15.00 plus mailing charges
2. Proceedings of the Full Board Meeting, July 1973, London, UK
January 1974 324pp. \$20.00 plus mailing charges

This supplies a useful summary of ICSU AB activities in 1972-3.

J. W. BARRETT

Official Representative of IUPAC to ICSU AB

COSTED TRAVEL FELLOWSHIPS

The Committee on Science and Technology in Developing Countries (COSTED) was set up by the XI General Assembly of ICSU, Bombay, on 10 January 1966, for the encouragement of science and technology in developing countries.

COSTED has instituted travel fellowships to assist scientists from the developing countries to participate in scientific seminars, *etc.* Details regarding the fellowships are given below. The funds available for the year 1974 are limited. However, it is hoped that with the satisfactory operation of the scheme this year, it will be possible to enhance this amount considerably in subsequent years.

Objectives

- (i) The travel fellowships are intended to enable scientists from developing countries to attend scientific conferences. Only those conferences where specific symposia are held will be considered for these awards. Attendance at General Assemblies will not be encouraged.
- (ii) The fellowships will also be available for scientists from developing countries to visit laboratories/institutions/industries for specialized training or project work or workshops.

Availability

- (i) The funds under this scheme will be available to support round trip international travel by economy class. The fare will be paid to the authorized travel agent.
- (ii) The fellowship does not include allowances for maintenance in the host country or break of journey en-route.

*Available from ICSU AB Secretariat, 17 Rue Mirabeau, F-75016 Paris, France

- (iii) There will be no restriction as to the country to be visited by the fellows.
- (iv) The fellowships will be available only for candidates from developing countries.
- (v) Fellowships will not be available for participation in programmes within the same country (e.g., Indians will not be eligible for a workshop in India).
- (vi) The fellowships will not be available for any programme which is of more than 3 months duration.

Applications

- (i) Only candidates below the age of 35 years will be eligible for these fellowships.
- (ii) Candidates should have a good academic background or industrial experience. These details should be included in the biodata attached to the applications.
- (iii) Candidates should normally be employed and should return to the position in the home country after the training.
- (iv) Candidates should establish availability of other sources of support for covering expenses during the stay abroad.
- (v) Candidates should have been accepted in the conference/project/workshop (this partly transfers the responsibility of judging the quality of the candidates to the sponsors).
- (vi) Two letters of assessment of the candidates should be sent directly to the COSTED Secretariat—one from a senior person in the field within the home country and the other, if possible, from the Director or Convenor of the conference/project/workshop.
- (vii) Applications should contain a statement (one page) of the likely benefits to the candidate in developing potential for future work in the home country.
- (viii) Applications should reach the COSTED Secretariat with supporting documents at least 3 months before the starting date of the programme.
- (ix) Applications should be addressed to the Scientific Secretary, COSTED Secretariat, Indian Institute of Science, Bangalore-560012, India.

Selection

Candidates selected for the awards will be intimated by the COSTED Secretariat.

APPENDICES TO IUPAC INFORMATION BULLETIN

The following Appendices were issued in August 1974:

Appendices on Provisional Nomenclature, Symbols, Units, and Standards

- No. 34. Proposed Terminology and Symbol for Transfer of Solutes from One Solvent to Another (Commission on Electroanalytical Chemistry)
- No. 35. Status of the Faraday Constant as an Analytical Standard (Commission on Electroanalytical Chemistry)
- No. 36. Recommendations on Usage of the Terms 'Equivalent' and 'Normal' (Commission on Analytical Nomenclature)
- No. 37. Recommendations for Nomenclature and Spectral Presentation in Chemical Electron Spectroscopy Resulting from Excitation by Photons (Commission on Molecular Structure and Spectroscopy)
- No. 38. Recommendations for the Presentation of NMR Data for Publication in Chemical Journals-B: Conventions Relating to Spectra from Other Nuclei (Commission on Molecular Structure and Spectroscopy)
- No. 39. Definitions, Terminology, and Symbols in Colloid and Surface Chemistry-II: Heterogeneous Catalysis (Commission on Colloid and Surface Chemistry)
- No. 40. Nomenclature of Corrinoids (IUPAC-IUB Commission on Biochemical Nomenclature)

Technical Reports

- No. 9. Recommended Method for Aflatoxins in Copra, Copra Meal, and Coconut (Section on Food)
- No. 10. Development of a Method to Evaluate Sampling Plans Used to Estimate Aflatoxin Concentrations in Lots of Shelled Peanuts (Section on Food)
- No. 11. Collaborative Study of the Determination of Aflatoxin M₁ in Milk (Section on Food)
- No. 12. Proposed Guidelines for Testing of Single Cell Protein Destined as Major Protein Source for Animal Feed (Section on Fermentation)
- No. 13. Report on International Education of Medicinal Chemists (Section on Medicinal Chemistry)

Subscribers to the *Information Bulletin* receive all Appendices automatically and free-of-charge on publication. Gratis copies may also be obtained by writing to:

Assistant Secretary (Publications)
IUPAC Secretariat
Bank Court Chambers
2-3 Pound Way
Cowley Centre
Oxford OX4 3YF, UK

For Appendices issued earlier, see *Information Bulletin* No. 47 (March 1974, page 39). Provisional (formerly Tentative) Nomenclature Appendices Nos. 1-17, 20-24, and 28-29, and Technical Reports Nos. 3-5 are now out of print.

Subject to the prior agreement of IUPAC, its provisional nomenclature recommendations may be:

- (a) Republished in other journals.
- (b) Translated into other languages through National Adhering Organizations.

NEW IUPAC PUBLICATIONS FROM BUTTERWORTHS

THE CONTRIBUTION OF CHEMISTRY TO FOOD SUPPLIES

This volume is a record of the invited papers, together with a limited number of the submitted papers, presented to the Symposium on 'The Contribution of Chemistry to Food Supplies' held in Hamburg during 29-31 August 1973. The Symposium was arranged jointly by the Food Section (acting on behalf of the Applied Chemistry Division) of IUPAC and IUFOST. It was the first joint Symposium to be arranged between these International Unions and was designed to establish areas of contact and cooperation in the very important fields of food production and food supplies. It presented an opportunity to bring together chemists, food scientists, and food technologists, from 24 countries and to focus attention on the contribution which each of these can bring to the other's problems.

The invited papers can be grouped into three areas, concerned respectively with chemical modifications to foods, food contaminants, and the development and evaluation of new proteins. The submitted papers are representative of a number of fields of new and developing technology and the symposium as a whole is of strong interest to those concerned with new or unconventional protein products.

viii+440 pages

\$18.00 or £6.00

EQUILIBRIUM CONSTANTS OF LIQUID-LIQUID DISTRIBUTION REACTIONS

Introduction and Part I: Organophosphorus Extractants

xiv+169 pages

\$15.00 or £5.00

Part II: Alkylammonium Salt Extractants

vii+85 pages

\$9.00 or £3.00

Compiled by Y. Marcus, A. S. Kertes, and E. Yanir

The Commission on Equilibrium Data of the Analytical Chemistry Division of the International Union of Pure and Applied Chemistry decided in 1963 to supplement the tables of *Stability Constants**, then going into a

**Stability Constants of Metal-Ion Complexes*, Second Edition, compiled by L. G. SILLÉN (inorganic ligands) and A. E. MARTELL (organic ligands), Chemical Society, London, Special Publication No. 17 (1964).

second edition, with constants for distribution equilibria of metal complexes. Extraction equilibria of both chelates and nonchelating systems were to be included. It soon transpired that the job of compiling these data was rather large, and also that the necessarily different organization of the material would make impractical the indiscriminate inclusion of these data in the Supplement to the second edition of Stability Constants, planned for publication in 1968 (later delayed to 1971). It was then decided that D. DYRSSEN and H. FREISER would take care of the compilation of data for chelating systems, while Y. MARCUS and A. S. KERTES would do the same for non-chelating ones.

An examination of the literature published in 1965 revealed that about three quarters of the relevant data deal with organophosphorus extractants. This was assumed to be the case for the period between 1955 and 1967, and also earlier these extractants constituted a large portion of those reported. Thus, a compilation of these data would be a significant portion of the whole effort, and it was decided to prepare it as a separate publication, in order to avoid finished work being unduly held up.

Very few papers with equilibrium constants for distribution reactions involving metal complexes were published prior to 1947. The literature search for the compilation therefore generally covers the period 1947-1968 inclusive. Some more recent publications (1969) are also included. For certain extractants, however, such as ethers and esters, significant publications are known to predate 1947. For these the literature search has started at as early a date as deemed suitable in each case.

It was decided that the compilation would be of greatest utility if it were limited to include only commonly used extractants, rather than try to include every system that has been reported in the literature. The aim, thus, is to obtain all the available information on a selected number of systems. It was found that for several organophosphorus extractants, although used in practical extraction work, no equilibrium constants have been reported, nor could they readily be obtained by the compilers from the original publications. Thus, the list of extractants which is actually presented is considerably shorter than the list which serves as the basis for the literature search.

Distribution equilibria involving metal ions often depend on other equilibria, involving the extractant and/or the inorganic ligand accompanying the metal ion. Thus, the partition of water, of acids and of the extractant itself are important reactions. So are also the equilibrium data on ionic dissociation of the extractant (mainly in the aqueous phase), its dimerization or further aggregation, and its association with other solvents. Therefore, in addition to the heterogeneous equilibria of the metal distribution, other heterogeneous and homogeneous equilibria which are relevant to the overall extraction reaction are also included in the compilation.

Part II consists of tables compiling equilibrium constants of distribution reactions involving extractants of the longchain alkylamine classes, primary, secondary, and tertiary, as well as quaternary ammonium salts, and other 'onium' salts: tetraphenylarsonium and tetraphenylphosphonium. The literature searched covers the period 1947-1969, with some of the more recent publications, 1970-1971, also included.

FIVE IMPORTANT NEW PUBLICATIONS AVAILABLE FROM IUPAC SECRETARIAT

Recommendations on Nomenclature for Chromatography

Nearly 10 years ago the Division of Analytical Chemistry approved a set of recommendations for the nomenclature of Gas Chromatography. Since then the Commission on Analytical Nomenclature has been endeavouring to produce a unified nomenclature applicable to all forms of separation processes, and proposals have been made for Liquid-Liquid Distribution and for Ion Exchange. In the present proposals,* prepared for the Commission by Dr. D. AMBROSE, Prof. E. BAYER, and Prof. O. SAMUELSON, the work has been extended to all forms of chromatography. For the sake of uniformity, compromises have inevitably had to be made, as a result of which, for example, there are some changes from the recommendations on Gas Chromatography. Account was taken, in the drafting, of other relevant proposals.

Published in *Pure and Applied Chemistry* (Vol. 37, No. 4, 1974) and available as a reprint (ii+16 pages) from the IUPAC Secretariat, price \$1.20 (£0.40) surface post or \$1.80 (£0.60) airmail.

Electrochemical Nomenclature

The present document constitutes Appendix III to the *Manual of Symbols and Terminology for Physicochemical Quantities and Units* [Butterworths: 1970 and *Pure Appl. Chem.* **21**, No. 1 (1970)] prepared by the Commission on Physicochemical Symbols, Terminology, and Units in 1969. It consists of recommendations for usage of symbols and terminology in electrochemistry. These recommendations are by no means complete and it is hoped that they will be supplemented in the future. The Commission on Electrochemistry has discussed these recommendations extensively† and in its deliberations has been greatly helped by comments received from many other interested scientists. These comments revealed considerable differences of opinion, and the recommendations presented here cannot reflect all preferences. However, the Commission hopes that these recommendations will be widely accepted and hence will serve to avoid some of the confusion which may exist as a result of different usages in electrochemistry.

Published in *Pure and Applied Chemistry* (Vol. 37, No. 4, 1974) and available as a reprint (ii+16 pages) from the IUPAC Secretariat, price \$1.20 (£0.40) surface post or \$1.80 (£0.60) airmail.

Quantities and Units in Clinical Chemistry

The Commission on Quantities and Units in Clinical Chemistry is a part of the Section on Clinical Chemistry of IUPAC. The Expert Panel on Quantities and Units is a part of the Committee on Standards of IFCC. These two bodies, the Commission and the Expert Panel, have worked on this document—the former mainly concerned with basic philosophy, the latter with problems of implementation.

*Issued first as Tentative Nomenclature Appendix No. 15 (February 1972) to *Information Bulletin*.

†Issued first as Tentative Nomenclature Appendix No. 28 (November 1972) to *Information Bulletin*.

The aim has been to have clinical chemical nomenclature become a natural part of the evolving international scientific language, especially by drawing upon the recommendations of the International Committee of Weights and Measures, IUB, Technical Committee 12 of ISO, and, of course, IUPAC.

The tentative version of the present publication appeared as Tentative Nomenclature Appendix No. 20 (February 1972) to the *Information Bulletin*. As a consequence of later decisions by international bodies concerned with nomenclature, a considerable number of comments, and new deliberations by the Commission and Expert Panel, this Recommendation 1973 contains many, mostly small modifications in comparison with the tentative version.

In cases of conflict, the present document supersedes the larger IUPAC-IFCC Recommendation 1966 and its translation into Spanish. *Recommendation 1966* was the first effort of international organizations towards a rationally standardized presentation of clinical chemical laboratory data. The present publication contains a revised condensation in Sections 3, 4, and 5 of R66. Chemical background material is given in Section 2. Section 6 corresponds to the R66 Part 5 with new kinds of quantities. Section 7 contains examples of clinical chemical quantities in a new generic form, which is further elaborated in a separate publication 'List of Quantities' (see below).

Published in *Pure and Applied Chemistry* (Vol. 37, No. 4, 1974) and available as a reprint (ii+28 pages) from the IUPAC Secretariat, price \$1.80 (£0.60) surface post or \$2.40 (£0.80) airmail.

List of Quantities in Clinical Chemistry

The aim of this document is to serve as a guide in supplanting present vernacular names for measurable properties in clinical chemistry. Systematic and more informative names are recommended, based on chemical and biochemical nomenclature. At the same time, a preference for 'molecular' kinds of quantities and SI units is stressed. The tentative version of the present publication appeared as Tentative Nomenclature Appendix No. 21 (February 1972) to the *Information Bulletin*.

Published in *Pure and Applied Chemistry* (Vol. 37, No. 4, 1974) and available as a reprint (ii+24 pages) from the IUPAC Secretariat, price \$1.80 (£0.60) surface post or \$2.40 (£0.80) airmail.

Atomic Weights of the Elements—1973

On the basis of work published, accepted for publication, or reevaluated from earlier publications, the Commission on Atomic Weights recommends changes in the atomic weight value for nickel and rhenium. In its 1973 Table the Commission has reverted to the former practice of listing the mass number of the isotope of longest half-life of certain radioactive elements instead of giving no indication of atomic weight value. The widespread use of separated stable isotopes of the rare gas elements is leading to the isotopically depleted material reaching commerce and a warning to users has been added for these elements. Also, the Commission emphasizes that the greatly increased use of fission-product materials and separated or enriched isotopic materials carries with it the danger that laboratory samples of anomalous isotopic composition could inadvertently be used.

Published in *Pure and Applied Chemistry* (Vol. 37, No. 4, 1974) and available as a reprint (ii+13 pages) from the IUPAC Secretariat, price \$0.90 (£0.30) surface post or \$1.35 (£0.45) airmail.

CALENDAR OF IUPAC-SPONSORED MEETINGS

1975

February 4-7	II International Congress on Industrial Waste Water and Wastes (Secretariat, II Congress on Industrial Waste Water and Wastes, POB 5607, S-114 86 Stockholm, Sweden)	Stockholm (Sweden)
June	Symposium on Polymerization of Heterocycles: Ring-Opening (Prof. St. PENCZEK, Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences, Ul. Przedzainiana 72, PL 90-339 Łódź, Poland)	Łódź-Jablonna (Poland)
July 1-4	IV Bratislava International Conference: Modified Polymers, Preparation and Properties (Dr. A. ROMANOV, Chairman of Organizing Committee, IV Bratislava International Conference on Modified Polymers, Polymer Institute, Slovak Academy of Sciences, Dúbravská Cesta, CS-809 34 Bratislava, Czechoslovakia)	Bratislava (Czechoslovakia)
July 6-11	25th IUPAC Congress (Organizing Committee, 25th IUPAC Congress, POB 983, Jerusalem, Israel)	Jerusalem (Israel)
July 13-18	International Symposium on Macromolecules (Secretariat, IUPAC Symposium on Macromolecules, Aharon Katzir-Katchalsky Center, Weizmann Institute of Science, Rehovot, Israel)	Jerusalem (Israel)
July 13-18	IX International Congress of Clinical Chemistry (Secretariat, IX International Congress of Clinical Chemistry, Toronto Dominion Centre, POB 34, Toronto, Ontario MK5 1B7, Canada)	Toronto (Canada)
July 21-25	XV Prague Microsymposium on Macromolecules: Degradation and Stabilization of Polyolefins (Organizing Committee, XV Prague Microsymposium on Macromolecules, Institute of Macromolecular Chemistry, Czechoslovak Academy of Sciences, Heyrovského Náměstí 2, CS-163 06 Praha 6, Czechoslovakia)	Prague (Czechoslovakia)
August 25-29	IV International Symposium on Carotenoids (Dr. H. PFANDER, Secretary General of Organizing Committee, IV International Symposium on Carotenoids, University Institute of Organic Chemistry, Länggass-Strasse 7, CH-3012 Berne, Switzerland)	Berne (Switzerland)
August 26-30	IV International Conference on Chemical Thermodynamics (Prof. M. LAFFITTE, Chairman of Organizing Committee, IV International Conference on Chemical Thermodynamics, Centre de Recherches de Microcalorimétrie et de Thermochimie, Centre National de la Recherche Scientifique, 26 Rue du 141 ^e RIA, F-13003 Marseille, France)	Montpellier (France)
September 2-11	28th IUPAC Conference: closed meeting of IUPAC bodies (Executive Secretary IUPAC, IUPAC Secretariat, Bank Court Chambers, 2-3 Pound Way, Cowley Centre, Oxford OX4 3YF, UK)	Madrid (Spain)
September 9-11	International Symposium on Marine Natural Products (Prof. R. H. THOMSON, Department of Chemistry, University of Aberdeen, Meston Walk, Old Aberdeen AB9 2UE, UK)	Aberdeen (UK)
September 12-16	Round Table on Study and Applications of Transport Phenomena in Thermal Plasmas (Prof. M. FOEX, Laboratoire des Ultra-Réfractaires, Centre National de la Recherche Scientifique, BP 5, Odeillo, F-66120 Font Romeu, France)	Font Romeu (France)

September 15-20	International Conference on Colloid and Surface Chemistry (Prof. E. WOLFRAM, Secretary of Organizing Committee, International Conference on Colloid and Surface Chemistry, Department of Colloid Science, Loránd Eötvös University, Puskin U. 11-13, H-1088 Budapest, Hungary)	Budapest (Hungary)
September- October	Symposium on Plasma Chemistry (Prof. H. SUHR, Chemisches Institut der Universität Tübingen, Auf der Morgenstelle, D-7400 Tübingen 1, Federal Republic of Germany)	Vienna (Austria)
1976		
May- June	V International Fermentation Symposium (Prof. H. DELLWEG, Chairman of Organizing Committee, V International Fermentation Symposium, Institut für Gärungsgewerbe und Biotechnologie, Seestrasse 13, D-1000 Berlin 65, Federal Republic of Germany)	Berlin (Federal Republic of Germany)
June	50th Anniversary Meeting of ACS Division of Colloid and Surface Chemistry (American Chemical Society, 1155 Sixteenth Street NW, Washington, DC 20036, USA)	Puerto Rico
July 12-16	VI International Congress on Catalysis (Dr. J. F. GIBSON, VI International Congress on Catalysis, Chemical Society, Burlington House, Piccadilly, London W1V 0BN, UK)	London (UK)
August 16-21	VIII International Symposium on Carbohydrate Chemistry (Prof. K. ONODERA, Department of Agricultural Chemistry, Kyoto University, Kyoto, Japan)	Kyoto (Japan)
August 23-28	X International Symposium on Chemistry of Natural Products (Mr. L. C. SOMERVILLE, Royal Society of New Zealand, 6 Halswell Street, POB 12-249, Wellington, New Zealand)	Dunedin (New Zealand)
September	III IUPAC Conference on Physical Organic Chemistry (Prof. G. LAMATY, Laboratoire de Chimie Organique Physique, Université des Sciences et Techniques du Langudoc, Place Eugène Bataillon, F-34060 Montpellier Cedex, France)	Montpellier (France)
1977		
September 4-10	26th IUPAC Congress (Prof. T. ASAHARA, Chairman of Preliminary Organizing Committee, Science Council of Japan, 22-23 Roppongi 7-chome, Minato-ku, Tokyo 106, Japan)	Tokyo (Japan)

CALENDAR OF NON-IUPAC MEETINGS

1975		
March 3-7	26th Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (Mr. A. T. WINSTEAD, American Chemical Society, 1155 Sixteenth Street NW, Washington, DC 20036, USA)	Pittsburgh (USA)
April 2-4	Colloque International sur les Matériaux de Substitution pour les Composants Électroniques (Secrétariat du Colloque, 16 Rue de Presles, F-75740 Paris Cedex 15, France)	Paris (France)

April 8-16	Symposium on Advances in Industrial Nitration Chemistry (Prof. L. F. ALBRIGHT, School of Chemical Engineering, Purdue University, Lafayette, Indiana 47907, USA; and Prof. C. HANSON, School of Chemical Engineering, University of Bradford, Bradford BD7 1DP, Yorkshire, UK)	Philadelphia (USA)
April 8-11	Reaktortagung 1975 (Deutsches Atomforum eV, Allianplatz, Haus X, D-5300 Bonn 1, Federal Republic of Germany)	Nürnberg (Federal Republic of Germany)
April 16-17	Application of Chemical Engineering to Treatment of Sewage and Industrial Liquid Effluents (Dr. D. GELDART, School of Chemical Engineering, University of Bradford, Bradford BD7 1DP, Yorkshire, UK)	York (UK)
May 5-7	I International Congress on Polymer Concretes [The Concrete Society (Congress), Terminal House, Grosvenor Gardens, London SW1W 0AJ, UK]	London (UK)
May 11-16	147th Meeting of Electrochemical Society (Mr. V. H. BRANNEKY, Assistant Executive Secretary, Electrochemical Society Inc., POB 2071, Princeton, New Jersey 08540, USA)	Toronto (Canada)
May 26-30	Colloque International sur l'Électronique et la Mesure (Secrétariat du Colloque, 16 Rue de Presles, F-75740 Paris Cedex 15, France)	Paris (France)
June 3-7	V International Conference on Atomic Masses and Fundamental Constants (Prof. P. GRIVET, AMCO-5, Institut d'Électronique Fondamentale, Bâtiment 220, Université Paris-Sud, F-91405 Orsay, France)	Paris (France)
June 17-20	27th International Meeting of Société de Chimie Physique: Lasers in Physical Chemistry (Dr. C. TROYANOWSKY, General Secretary, Société de Chimie Physique, 10 Rue Vauquelin, F-75231 Paris Cedex 05, France)	Paris (France)
June 18-20	Colloque International sur la Fiabilité et la Disponibilité des Systèmes Informatiques (Secrétariat du Colloque, 16 Rue de Presles, F-75740 Paris Cedex 15, France)	Paris (France)
June 24- July 3	IV International Summer Conference: Chemistry of Solid-Liquid Interfaces (Dr. V. PRAVDIC, Rudjer Bošković Institute, POB 1016, YU-41001 Zagreb, Yugoslavia)	Cavtat- Dubrovnik (Yugoslavia)
July 29- August 6	International Conference on Improvement of Physics Education (Dr. R. M. SILLITO, Department of Physics, University of Edinburgh, Mayfield Road, Edinburgh, UK)	Edinburgh (UK)
August 7-15	X General Assembly and International Congress of Crystallography (Congress Organizing Committee, POB 7205, Amsterdam, Netherlands)	Amsterdam (Netherlands)
August 24-29	5th International Congress of Chemical Engineering, Chemical Equipment, Design, and Automation (Secretariat, 5th CHISA-Congress, POB 857, Praha 1, Czechoslovakia)	Prague (Czechoslovakia)
August 25-30	II European Conference on Analytical Chemistry (EUROANALYSIS II, c/o Hungarian Chemical Society, POB 240, H-1368 Budapest, Hungary)	Budapest (Hungary)
August 25-29	V International Conference on Atomic Spectroscopy (Dr. J. B. WILLIS, Secretary, V International Conference on Atomic Spectroscopy, CSIRO Division of Chemical Physics, POB 160, Clayton, Victoria, Australia 3168)	Clayton- Melbourne (Australia)

August 25 –September 6	XVI General Assembly of International Union of Geodesy and Geophysics (Comité National Français de Géodésie et Géophysique, 136 bis, Rue de Grenelle, F-75700 Paris, France)	Grenoble (France)
September 1–5	II World Conference on Computers in Education (Mr. J. HEBENSTREIT, École Supérieure d'Électricité, 10 Avenue Pierre-Larousse, F-92240, Malakoff, France)	Marseille (France)
September 3–5	6th Symposium on Industrial Crystallization (Ing. R. RYCHLÝ, Forschungsinstitut für Anorganische Chemie, Postfach 176, CS-400 60 Usti nad Labem, Czechoslovakia)	Usti nad Labem (Czechoslovakia)
September 9–12	II International Symposium on Tests on Bitumins and Bituminous Materials (Symposium Secretariat, Hungarian Chemical Society, Anker Kőz 1, H-1061 Budapest, Hungary)	Budapest (Hungary)
September 15–19	XVIII Colloquium Spectroscopicum Internationale (Prof. G. EMSCHWILLER, 8–10 Rue du Delta, Paris IX, France)	Grenoble (France)
September 15–19	4th European Symposium on Corrosion Inhibitors (Secretariat, 4 SEIC, Istituto Chimico, University of Ferrara, Via Scandiana 25, I-44100 Ferrara, Italy)	Ferrara (Italy)
September 17–20	Conference on Polymer Rheology and Plastics Processing (Plastics Institute, 11 Hobart Place, London SW1W 0HL, UK)	Loughborough (UK)
September 21–26	26th Meeting of International Society of Electrochemistry: Electrochemistry of Nonaqueous Solvents (Dr. H. TANNENBERGER, Secretary General ISE, Battelle Centre de Recherche de Genève, 7 Route de Drize, CH-1227 Carouge-Genève, Switzerland)	Vienna (Austria)
September 24–26	6 Europäisches Symposium 'Lebensmittel—Physikalische und Mechanische Verfahren bei der Lebensmittelverarbeitung unter besonderer Berücksichtigung der Lebensmittelqualität' (Dr. R. JOWITT, National College of Food Technology, St. George's Avenue, Weybridge, Surrey, UK)	Cambridge (UK)
September	Symposium on Transplutonium Elements and Plutonium Ceramic Materials (Prof. W. MÜLLER, European Institute of Transuranium Elements, Kernforschungszentrum Karlsruhe, Postfach 22600, D-7500 Karlsruhe, Federal Republic of Germany)	Baden-Baden (Federal Republic of Germany)
October 7–11	4th International Nuclear Industries Fair and Technical Meetings (Secretariat NUCLEX 75, Swiss Industries Fair, CH-4000 Basel 21, Switzerland)	Basel (Switzerland)
December 3–9	VI International Congress on Metallic Corrosion (Conference Secretary, VI International Congress on Metallic Corrosion, POB 391, Darlinghurst, New South Wales, Australia 2010)	Sydney (Australia)

LIST OF ABBREVIATIONS

ACHEMA	Ausstellungstagung für Chemisches Apparatewesen
ACS	American Chemical Society
AFNOR	Association Française de Normalisation

(continued on inside back cover)

International Union of Pure and Applied Chemistry

Standard Methods for Analysis of Oils Fats & Soaps

3rd Supplement

1974. 36 pages. \$2.40 (£0.80) 0 408 70567 1

The 3rd supplement to the Standard Methods of the IUPAC Oils and Fats Section contains the texts of six additional methods of analysis that are applicable to the study of oils, fats and soaps.

Just as the previous publications, this supplement was achieved by the combined efforts of the members of the Section. The methods in question were investigated by means of collaborative tests, on the basis of which the definitive texts were drawn up and finally adopted.

The purpose is to supply standard methods for the analysis of oils, fats, soaps and other oleochemicals that can be used internationally, e.g. in quality control, general research, commerce and industry. In this connection, new methods corresponding to current needs, modern trends and progress in analytical chemistry and technology, are constantly being studied by the Oils and Fats Section and, if approved, they are added to the list of those already published.

Also available:—

First supplement \$7.50 (£2.50) 118 pages

Second „ \$7.50 (£2.50) 30 pages 0 408 70427 6

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International Union of Pure and Applied Chemistry

INTERNATIONAL THERMODYNAMIC TABLES—ETHYLENE

Editor: S. Angus

This book is the second of a series which is intended to display in tabular form the best available values of the thermodynamic properties of fluids of scientific and industrial importance.

The tables given are constructed according to the advice of an international panel of experts in the field on the basis of correlations of the properties of ethylene made by workers in the U.K., with considerable help from other workers in France, the USA and the USSR. The completed tables have been approved by a wide range of thermodynamicists, including the IUPAC Commission on Thermodynamics and Thermochemistry.

The properties are expressed in tabular form because it is the numbers which have international approval: they can in theory be reproduced by many equations, and one set which will do this is given.

The properties listed are density, internal energy, entropy, enthalpy, the heat capacities, the compression factor, fugacity and speed of sound, some on a pressure-temperature basis and some on a density-temperature basis. Orthodox saturation tables are also given, as are the ideal gas and zero pressure properties.

1974. 232 pages. \$36.00 (£12.00) 0 408 70555 8

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425 K

TOLERANCE DIAGRAM. SPECIFIC VOLUME

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AIP	American Institute of Physics
AIPEA	Association International pour Étude Agricole
AOAC	Association of Official Analytical Chemists
ASIDIC	Association of Scientific Information Dissemination Centres in USA
CBN	IUPAC-IUB Commission on Biochemical Nomenclature
CCS	IUPAC Clinical Chemistry Section
CEE	Communauté Européenne Economique
CIA	CID Commission Internationale d'Analyses
CID	Comité International des Dérivés Tensio-Actifs
CIE	CID Commission Internationale d'Essais
CIHAA	Commission Internationale des Industries Agricole et Alimentaires
CIT	CID Commission Internationale de Terminologie
CNRS	Centre National de la Recherche Scientifique in France
CODATA	ICSU Committee on Data for Science and Technology
COSPAR	ICSU Committee on Space Research
COSTED	ICSU Committee on Science and Technology in Developing Countries
CQUCC	IUPAC Commission on Quantities and Units in Clinical Chemistry
EP on QU	Expert Panel on Quantities and Units of IFCC Committee on Standards
EUSIDIC	European Association of Scientific Information Dissemination Centres
FAO	UN Food and Agriculture Organization
FECS	Federation of European Chemical Societies
FDA	US Food and Drug Administration
GARP	Global Atmospheric Research Programme
IARC	WHO International Agency for Research on Cancer
IAU	International Astronomical Union
IAWPR	International Association on Water Pollution Research
ICC	International Association for Cereal Chemistry
ICSU	International Council of Scientific Unions
ICSU AB	ICSU Abstracting Board
IFCC	International Federation of Clinical Chemistry
IGU	International Geographical Union
ILO	UN International Labour Organization
IMA	International Microbiological Association
INSPREC	Information Services for Physics, Electrotechnology, and Control
ISE	International Society of Electrochemistry
ISO	International Organization for Standardization
IUB	International Union of Biochemistry
IUBS	International Union of Biological Sciences
IUCr	International Union of Crystallography
IUFoST	International Union of Food Science and Technology
IUGG	International Union of Geodesy and Geophysics
IUGS	International Union of Geological Sciences
IUNS	International Union of Nutritional Sciences
IUPAB	International Union of Pure and Applied Biophysics
IUPAP	International Union of Pure and Applied Physics
IUPHAR	International Union of Pharmacology
IUPS	International Union of Physiological Sciences
IUTAM	International Union of Theoretical and Applied Mechanics
MEDLARS	Medical Literature Analysis and Retrieval System
NBS	US National Bureau of Standards
PAG	Protein Advisory Group of FAO/WHO/UNICEF
RILEM	Réunion Internationale des Laboratoires d'Essais et de Recherches sur les Matériaux et les Constructions
SCAR	ICSU Scientific Committee on Antarctic Research
SCIBP	ICSU Special Committee for the International Biological Programme
SCOPE	ICSU Scientific Committee on Problems of the Environment
SCOR	ICSU Scientific Committee on Oceanic Research
SI	Système International
UKCIS	UK Chemical Information Service
UN	United Nations
UNEP	UN Environment Programme
UNESCO	UN Educational, Scientific, and Cultural Organization
UNICEF	UN Children's Fund
UNISIST	UNESCO-ICSU Programme on International Science Information System
WFEQ	World Federation of Engineering Organizations
WHO	UN World Health Organization

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**INTERNATIONAL UNION OF PURE
AND APPLIED CHEMISTRY**

**INFORMATION BULLETIN
NUMBER 49**

MARCH 1975

IUPAC SECRETARIAT

Bank Court Chambers, 2/3 Pound Way
Cowley Centre, Oxford OX4 3YF, UK

Telephone—Oxford 770125 & 772834
Telegrams—IUPAC OXFORD

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International Union of Pure and Applied Chemistry
1975

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

President —Prof. Sir HAROLD THOMPSON (UK)
Vice-President —Dr. R. W. CAIRNS (USA)
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IUPAC INFORMATION BULLETIN

The Bulletin provides a news medium for the various activities of IUPAC, especially of its 50 or so committees which deal with chemical topics needing regulation, standardization or codification. It carries advance information on forthcoming symposia which are to be sponsored by IUPAC together with reports of such meetings which have recently taken place. Coverage is also given to projects in which IUPAC is collaborating with other international organizations.

Two series of Appendices to the Bulletin are issued:

- (i) Appendices on Provisional Nomenclature, Symbols, Units, and Standards
- (ii) Technical Reports

In 1975 there will be two issues (Nos. 50 and 51). Annual subscription to the Bulletin, inclusive of the two series of Appendices and postal charges, is US \$12.00 or £4.00 (surface); US \$22.50 or £7.50 (Bulletin and Appendices by air); US \$19.50 or £6.50 (Bulletin by surface and Appendices by air); US \$16.00 or £5.33 (Bulletin by air and Appendices by surface).

Subscription orders may be placed direct, or through an agent, with the IUPAC Secretariat.

To all our Readers

Extracts from the *Information Bulletin* may be reproduced freely in university bulletins, industrial house magazines, information newsheets, and national journals. In particular, IUPAC will be pleased for attention to be drawn to the availability of its new publications and to the dates and subjects of forthcoming international symposia of the Union.

28th IUPAC Conference

MADRID, 2—11 SEPTEMBER 1975

Key to Map Overleaf

X — Hotel Meliá Castilla

Consejo Superior Investigaciones de Científicas (Madrid-6):

A — Edificio Central, Serrano 117

B — Instituto de Química Física 'Rocasolano', Serrano 119

C — División de Ciencias, Serrano 113

D — Centro Nacional de Química Orgánica, Juan de la Cierva 3

E — Instituto de Edafología y Fisiología Vegetal, Serrano 115 bis

F — Patronato 'Juan de la Cierva', Serrano 150

G — Centro de Investigaciones Biológicas, Velázquez 114

City of Madrid



28th IUPAC CONFERENCE*

MADRID, 2-11 SEPTEMBER 1975

Accommodation and Travel

Full details of accommodation reserved at Hotel Meliá Castilla (Calle del Capitán Haya 37, Madrid-20) and various travel schemes have been distributed to National Adhering Organizations, to Associated Organizations, and to Titular and Associate Members and National Representatives of IUPAC bodies. Any queries should be addressed to the IUPAC Secretariat. There will be an IUPAC information desk at Madrid airport.

Visas

Conference participants are recommended to check at the Spanish Embassy in their respective countries on the necessity of obtaining a visa to travel to Madrid. An official letter supporting a visa application may be obtained from the IUPAC Secretariat.

Schedule of Meetings

Subject to last minute changes, the Schedule of Meetings is as shown on pages 3-10. All meetings will be held at Institutes of the Consejo Superior Investigaciones de Científicas. Details of provisional meeting rooms and times of meetings are included in the Schedule. It is hoped to arrange transport between the Hotel and the Institutes during the Conference.

Lord TODD, a former President of IUPAC, has been invited to address the Conference participants. His lecture

Chemistry in a Changing World—A Look Ahead

will be at 1900 hours on 10 September. Also, there will be two symposia on chemical education (see page 125 for further details):

- (i) 6-7 September *Educational Technology in the Teaching of Chemistry* organized by the IUPAC Committee on Teaching of Chemistry
- (ii) 7-8 September *Chemical Education in Europe—New Approaches* organized by FECS

Several international symposia sponsored by IUPAC are due to take place in Europe immediately before or after the Conference (see pp. 134-135).

Secretariat

Throughout the Conference the IUPAC Secretariat will be located in the Edificio Central del Consejo Superior Investigaciones de Científicas (Serrano 117): telephone 2-61-98-00. The Secretariat will be open daily and provide typing, photocopying, and other services to assist Conference participants in their work.

Registration will take place at the Secretariat and not in the Meliá Castilla.

*Attendance restricted to elected Members of IUPAC bodies, National Representatives, and Delegates of Associated Organizations.

Social Programme

The Spanish National Committee of IUPAC hopes to arrange some social functions. It is hoped also to arrange a Conference Dinner in the Meliá Castilla on the evening of 10 September following the lecture by Lord TODD. The cost of the Dinner will be about 600 pesetas (inclusive of wine) per person. A Ladies Programme is being planned.

Weather and Clothing

The average temperature at the start of September in Madrid is 28°C. Formal dress will not be essential for any of the social functions.

SCHEDULE OF MEETINGS FOR 28th IUPAC CONFERENCE

(*Denotes Joint Meeting)

Meeting of	Tuesday 2 September	Wednesday 3 September	Thursday 4 September	Friday 5 September	Saturday 6 September	Sunday 7 September	Monday 8 September	Tuesday 9 September	Wednesday 10 September	Thursday 11 September
Council								10-12.30 15-18		
Bureau							9-12(A2) 15-18(A2)			
Executive Committee						9-12(A2) 15-18(A2)				15-17(A2)
Division Presidents				18-20(A3)						17-19(A2)
Committee on Publications	9-12(A3) 15-18(A3)									
Committee on Teaching of Chemistry		9-12*(G3) 15-18*(B1)	9-12*(C3) 15-18(C3)	9-12(A2) 15-18(A2)						
Coordinating Committee for Analytical Methods					17-20*(F5)					
Finance Committee					9-12(A3) 15-18(A3)					
Interdivisional Committee on Machine Documentation	9-12(A3) 15-18(A3)	9-12(A3) 15-18(A3)	9-12(A3) 15-18(A3)							
Interdivisional Committee on Nomenclature and Symbols	15-18(B3)					15-18(B3)				
Interdivisional Open Meeting on Data Flagging		18-20(E3)								
Coordinating Committee and Section VI.1					17-20*(F4)					
Committee on Teaching of Chemistry (Officers) and Commission on Teaching in Clinical Chemistry			9-12*(G3)							

Meeting of	Tuesday 2 September	Wednesday 3 September	Thursday 4 September	Friday 5 September	Saturday 6 September	Sunday 7 September	Monday 8 September	Tuesday 9 September	Wednesday 10 September	Thursday 11 September
Committee on Teaching of Chemistry (Officers), Inorganic Chemistry Division Committee, and Commissions II.1 and I.1		15-18*(B1)								
Committee on Teaching of Chemistry (Officers) and Commission V.7			9-12*(C3)							
Clinical Chemistry Section										
Section Committee							9-12(G1) 15-18(G1)			
Commission on Automation			9-12(B2) 15-18(B2)	9-12(B2) 15-18*(E6)	9-12(B2) 15-18(B2)					
Commission on Quantities and Units		9-12(G1) 15-18(G1)	9-12(G1) 15-18(G1)	9-12(G1) 15-17*(B1)	9-12(G1) 15-18(G1)					
Commission on Teaching		9-12*(G3)	9-12(G3) 15-18(G3)	9-12(G3) 15-18(G3)						
Commission on Toxicology			9-12(G2) 15-18(G2)	9-12(G2) 15-18(G2)	9-12(G2) 15-18(G2)					
Clinical Chemistry Section (Officers) and Clinical Chemistry Commissions (Chairmen)			15-18(G1)							
Commission on Automation and Commission V.3							15-18*(E6)			
Commission on Quantities and Units and Commission I.1							15-17*(B1)			
Commission on Teaching in Clinical Chemistry and Committee on Teaching of Chemistry (Officers)				9-12*(G3)						

Meeting of	Tuesday 2 September	Wednesday 3 September	Thursday 4 September	Friday 5 September	Saturday 6 September	Sunday 7 September	Monday 8 September	Tuesday 9 September	Wednesday 10 September	Thursday 11 September
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Physical Chemistry Section

Division Committee	9-12(B5) 15-18(B5)		15-18*(B5)			9-12(B5) 15-18(B5)				
Commission I.1: Physicochemical Symbols, Terminology, and Units	9-12(B1) 15-18*(B1)	9-12(B1) 15-18(B1)	9-12(B1) 15-18(B1)	9-12*(B1) 15-17*(B1) 17-19*(B1)	9-12*(B1) 15-18(B1)	9-12*(B1) 15-18(B1)				
Commission I.2: Thermodynamics and Thermochemistry	9-12(D4) 15-18(D4)			9-12*(D4) 15-17*(D4) 17-19*(B1)	9-12(D4) 15-18(D4)	9-12(D4) 15-18(D4)				
Sub-Commission I.2.1: Plasma Chemistry			9-12(D4) 15-18(D4)	9-12(B3) 15-17*(D4)						
Sub-Commission I.2.2: Thermodynamic Tables			9-12(B7) 15-18(B7)	9-12*(D4)						
Commission I.3: Electrochemistry	9-12(B4) 15-18(B4)		9-12*(B5)	9-12(B4) 15-18*(B3)	9-12(B4) 15-18(B4)					
Commission I.4: Physicochemical Measurements and Standards	9-12(B5)			9-12(B5)	9-12(B5)					
Sub-Commission I.4.1: Calibration and Test Materials	15-18(B5)		9-12(B3)	15-18(B5)						
Commission I.5: Molecular Structure and Spectroscopy	9-12(B6) 15-18(B6)		9-12(B6)	9-12(B6) 15-18(B6)	9-12*(B1) 15-18(B6)					
Commission I.6: Colloid and Surface Chemistry	9-12(B3) 15-16*(B3) 16-18(B3)		9-12*(B5)	9-12*(B1) 15-18*(B3)	9-12*(D3) 15-18(B3)					
Division Committee and Commissions (Officers)				15-18*(B5)						

Meeting of	Tuesday 2 September	Wednesday 3 September	Thursday 4 September	Friday 5 September	Saturday 6 September	Sunday 7 September	Monday 8 September	Tuesday 9 September	Wednesday 10 September	Thursday 11 September
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Physical Chemistry Division (continued)

Commission I.1 and Commission on Quantities and Units in Clinical Chemistry				15-17*(B1)						
Commission I.1 and I.2				17-19*(B1)						
Commissions I.1 and I.5					9-12*(B1)					
Commissions I.1 and I.6				9-12*(B1)						
Commissions I.1 and II.1, Committee on Teaching of Chemistry (Officers), and Inorganic Chemistry Division Committee			15-18*(B1)							
Commission I.2 and Sub-Commission I.2.1				15-17*(D4)						
Commission I.2 and Sub-Commission I.2.2				9-12*(D4)						
Commissions I.3 and I.6			9-12*(B5)							
Commissions I.3 and V.5				15-18*(E3)						
Commission I.6 and Commission II.2 (Chairman only)		15-16*(B3)								
Commissions I.6 and IV.1					9-12*(D3)					

Inorganic Chemistry Division

Division Committee	9-12*(C1) 15-18(C1)	15-18*(C1)				9-12*(C1) 15-18(C1)				
Commission II.1: Atomic Weights		9-12(C1) 15-18*(B1)	9-12(C1) 15-18(C1)	9-12(C1) 15-18(C1)	9-12(C1) 15-18(C1)					

Meeting of	Tuesday 2 September	Wednesday 3 September	Thursday 4 September	Friday 5 September	Saturday 6 September	Sunday 7 September	Monday 8 September	Tuesday 9 September	Wednesday 10 September	Thursday 11 September
Commission II.3: High Temperatures and Refractory Materials		9-12(C2) 15-18(C2)	9-12(C2)	9-12(C2) 15-18(C2)	15-18(C2)					
Division Committee, Committee on Teaching of Chemistry (Officers), and Commissions I.1 and II.1		15-18*(B1)								
Commission II.2 (Chairman only) and Commission I.6		15-16*(B3)								
Division Committee and Commissions (Chairmen)	9-12*(C1)					9-12*(C1)				
Organic Chemistry Division										
Division Committee		9-12(D1) 15-18*(D1)			9-12(D2) 15-18(D2)	9-12(D1) 15-18(D1)				
Commission III.1 (Chairman only)		15-18*(D1)								
Commission III.3: Organic Photochemistry			9-12(D5) 15-18(D5)	9-12(D5) 15-18(D5)						
Section III.4: Medicinal Chemistry			9-12(D1) 15-18(D1)	9-12(D1) 15-18(D1)	9-12(D1)					
Division Committee and Commissions/ Section (Chairmen only)		15-18*(D1)								
Division Open Meeting					15-18(D2)					
Macromolecular Division										
Division Committee	9-12(D3)					15-18(D3)				

Meeting of	Tuesday 2 September	Wednesday 3 September	Thursday 4 September	Friday 5 September	Saturday 6 September	Sunday 7 September	Monday 8 September	Tuesday 9 September	Wednesday 10 September	Thursday 11 September
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Commission IV.1: Macromolecular Nomenclature	15-18(D3)	9-12(D3) 15-18(D3)	9-12(D3) 15-18(D3)	9-12(D3) 15-18(D3)	9-12*(D3)					
Commissions IV.1 and I.6					9-12*(D3)					

Analytical Chemistry Division

Division Committee	9-12(E3) 15-18(E3) 18-19*(F1)	10-12(E5)			15-17(E1)	9-12*(E3) 15-17*(E3) 17-19(E3)				
Commission V.1: Analytical Reactions and Reagents		15-17*(E1)	9-12(E2) 15-18(E2)	9-12(E2) 15-18(E2)						
Commission V.2: Microchemical Techniques and Trace Analysis			9-12(E5) 15-18(E5)	9-12(E5) 15-18(E5)	9-12(E5)					
Commission V.3: Analytical Nomenclature		10-12(E6)	9-12*(E6) 15-18(E6)	9-12*(E3) 15-18*(E6)	9-12(E6)					
Commission V.4: Spectrochemical and Other Optical Procedures for Analysis		10-12(F5)	9-12*(E6) 15-18(F5)	9-12(F5) 15-18(F5)	9-12(F5)					
Commission V.5: Electroanalytical Chemistry		10-12(E4)	9-12(E4) 15-18(B1)	9-12(E3) 15-18*(E3)	9-12(E3)					
Commission V.6: Equilibrium Data		10-12(E3) 15-18(E3)	9-12(E3) 15-18(E3)	9-12(E4) 15-18(E4)	9-12*(E3)					
Sub-Commission V.6.1: Solubility Data	9-12(E3) 15-18(E3)									
Commission V.7: Analytical Radiochemistry and Nuclear Materials		10-12(C3)	9-12*(C3)	9-12(C3) 15-18(C3)	9-12(C3)					

Meeting of	Tuesday 2 September	Wednesday 3 September	Thursday 4 September	Friday 5 September	Saturday 6 September	Sunday 7 September	Monday 8 September	Tuesday 9 September	Wednesday 10 September	Thursday 11 September
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Analytical Chemistry Division (continued)

Division Committee (Secretary) and Commissions (Secretaries)	9-10*(E3)									
Division Committee and Commissions (Chairmen)	9-12*(E3) 15-17*(E3)									
Division Committee and Applied Chemistry Division Committee	18-19*(F1)									
Division Open Meeting	15-17*(E1)									
Commission V.1 and Section VI.1	15-17*(E1)									
Commission V.3 and Commission on Automation in Clinical Chemistry	15-18*(E6)									
Commissions V.3 and V.4	9-12*(E5)									
Commissions V.5 and I.3	15-18*(E3)									
Commission V.7 and Committee on Teaching of Chemistry (Officers)	9-12*(C3)									

Applied Chemistry Division

Division Committee	10-12.30(F1) 15-18*(F1) 18-19*(F1)	14-16(E1) 16-17(E1) 17-18*(E1)	10-12(F1) 15-18(F1)
Section VI.1: Food	9-10(F1) 9-12(F5) 15-17*(E1) 17-19*(E1)	17-19*(E1) 19-20*(F3)	9-12(F5) 17-20*(F5)
Commission VI.1.1.: Food Additives	10-12(F6) 15-18(F6)	9-12(F6) 15-17(F6)	9-12(F6)
Commission VI.1.2: Food Contaminants	10-12(F7) 15-18(F7)	9-12(F7) 15-17(F7)	9-12(F7)
Section VI.2: Fermentation	9-12(F9) 15-17(F9) 17-19*(E1)	9-12(F9) 15-18(F9)	9-12*(F9)

Meeting of	Tuesday 2 September	Wednesday 3 September	Thursday 4 September	Friday 5 September	Saturday 6 September	Sunday 7 September	Monday 8 September	Tuesday 9 September	Wednesday 10 September	Thursday 11 September
Applied Chemistry Division (continued)										
Section VI.3: Oils and Fats		15-17(F1)	9-12(E1) 15-16(E1) 16-17*(E1) 17-19*(E1)	9-12(F1)	9-12(F1) 15-18(F1)					
Section VI.4: Air Quality		9-12(F2) 15-18(F2)	9-12(F2) 15-18(F2)	9-12(F2)						
Section VI.5: Pesticides	9-12(F3)	9-12(F3) 15-18(F3)	9-12(F3) 16-17*(E1) 19-20*(F3)		10-12(F3) 15-18(F3)					
Commission VI.5.1: Terminal Pesticide Residues		9-12(F3) 15-18(F3)	9-12(F3) 17-19(F3)		15-18(F3)					
Commission VI.5.2: Pesticide Residue Analysis		9-12(F3) 15-18(F3)		9-12(F3) 18-20(F3)	15-18(F3)					
Section VI.6: Water Quality			9-12(E7) 15-18(E7)	9-12*(F9)	9-12(E7) 15-18(E7)					
Division Committee and Sections (Officers)	15-18*(F1)			17-18*(E1)						
Division Committee and Analytical Chemistry Division Committee	18-19*(F1)									
Division Open Meeting				14-16(E1)						
Section VI.1 and Coordinating Committee					17-20*(F5)					
Section VI.1 and Commission V.1		15-17*(E1)								
Sections VI.1 and VI.2		17-19*(E1)								
Sections VI.1 and VI.3			17-19*(E1)							
Sections VI.1 and VI.5			19-20*(F3)							
Sections VI.2 and VI.6				9-12*(F9)						
Sections VI.3 and VI.5			16-17*(E1)							

ATTENDANCE AT SYMPOSIA SPONSORED BY IUPAC

At a meeting of the Bureau held in Brussels on 31 August-1 September 1974, a number of cases were reported in which *bona fide* chemists from member countries of IUPAC had been prevented from attending symposia sponsored by the Union in 1974 through a refusal to grant entry visas. IUPAC has always upheld firmly the principle of such freedom to participate in its meetings. Prior to the granting of sponsorship, the Union as normal practice seeks an assurance from the organizers that *bona fide* chemists from throughout the world will be admitted to the country where a symposium is to be held.

After careful consideration of these matters, the Bureau has resolved that whenever possible the submission of applications for entry visas where necessary should be made to the appropriate authorities not less than three months prior to an IUPAC-sponsored symposium. If visas are then not granted or promised in writing one month before the date of the meeting and the applicants inform IUPAC giving all details, sponsorship may be withdrawn by the Union. The main invited lecturers will then be informed of any such decision and other meetings under the auspices of IUPAC in the country concerned will be suspended until more satisfactory circumstances exist.

The procedure now to be adopted by IUPAC was mentioned at the 15th General Assembly of ICSU (Istanbul, 23-26 September 1974) and by an overwhelming majority it was recommended for observance by other International Scientific Unions and by ICSU.

H. W. THOMPSON
President

"PREDICTED" COMPOUNDS WITH "ALLEGED" BIOLOGICAL ACTIVITIES FROM ANALYSES OF STRUCTURE- ACTIVITY RELATIONSHIPS*

IMPLICATIONS FOR MEDICINAL CHEMISTS

Introduction

Until recently, structure-activity relationships in series of bioactive compounds have been defined largely in descriptive terms. The last decade has, however, seen some particularly rapid developments in the use of stereochemical and physicochemical parameters, molecular orbital calculations, *etc.*, which, in conjunction with computer-assisted regression analyses, have permitted quantitative descriptions of structure-activity relationships.† Analyses of these results have permitted deeper understandings of structure-activity relationships and speculations regarding mechanisms of drug actions.

It is recognized that the scientists responsible for these developments in quantitative structure-activity relationships have made a major contribution to medicinal chemistry and have opened new vistas in our understanding of the relationships between chemical structure and biological activity.

Of relevance to this report is that these newer methods have permitted the design of chemical structures which are predicted to have a specific biological activity. Unfortunately, few of these predictions have been tested experimentally and it is the purpose of this report to examine some of the consequences of the very existence of methods so powerful that they permit the prediction of structures which are alleged to have a specific biological activity. Some of these consequences, particularly effects on patentability, which are described in some detail, tend to discourage the synthesis and testing of predicted compounds. Some specific recommendations are made which should serve instead to encourage this completion of the scientific method, the verification of hypotheses.

Consequences Relating to Patentability

In this area, the *ad hoc* Committee has considered the following question: "What is the patentability of a compound which hitherto had not been synthesized, but which had previously been publicly predicted to possess a specific biological activity?"

If the sophisticated analyses of structure-activity relationships as currently practiced were capable of predicting only structures which were closely related to the prototypes from which they were derived, there would be no need for this report, because such structures would be regarded as being obvious and therefore not patentable over the relevant prior art. The methods available are, however, considerably more versatile. Appendix B lists the structures of fifteen compounds which have been predicted, during the

*Report prepared by an *ad hoc* Committee of the Section on Medicinal Chemistry: Dr. L. G. HUMBER (Chairman), Prof. A. ALBERT, Prof. E. CAMPAIGNE, Dr. J. F. CAVALLA, Dr. NITYA ANAND, Dr. M. PROTIVA, Dr. A. I. RACHLIN, Prof. P. SENSI.

†It is assumed that readers of this report are familiar with the methods referred to and therefore no attempt has been made either to describe or to evaluate these methods. They have been critically reviewed frequently in the recent past (see Appendix A).

period 1963-1971, to possess various biological activities. This Appendix includes references, the specific alleged biological activity, as well as the structural prototypes from which they have been derived. While individual judgements may vary as to whether a given predicted structure is "closely related" and thus "obvious" over the prototype from which it is derived, the *ad hoc* Committee considers that the majority of the predicted structures shown in Appendix B (e.g., VI-VIII, X-XV) differ substantially from the prototypes that have led to their prediction. These examples, then, are instances where theoretical means have led to the prediction of novel classes of compound which are alleged to have specific biological properties.

Unfortunately, none of the structures shown in Appendix B has ever been synthesized, as judged by exhaustive searches of *Chemical Abstracts* and the *Ringdoc Abstracts* to November 1973. In the absence of predictions of biological activities, the actual syntheses of these compounds along with demonstrations of "utility", would undoubtedly result in the granting of patent protection in numerous countries.

It will be instructive to consider how the patentability of such compounds is prejudiced by a prior prediction that these structures possess a specific biological activity. The types of patent protection available for pharmaceuticals differ from one country to the other and, with respect to the type of protection available, each country may have quite different guidelines. It is not the intention of the *ad hoc* Committee to review in this report the patent laws of each country. Generally, four types of patent protection for pharmaceuticals are available: (a) "Product" patents, in which the chemical substance *per se* is patented; (b) "Process" patents, in which the process for manufacturing the chemical substance is patented; (c) "Pharmaceutical Composition" patents, in which a patent is granted for a pharmaceutical formulation containing the chemical substance as the active ingredient; (d) "Method of Treatment" patents, in which a method of therapeutically treating humans with a pharmaceutical product is covered.

Not all countries grant all of the above types of patent protection. As a guide, the reader is referred to Appendix C which summarizes the type or types of patent protection available for pharmaceuticals in various countries. In the following paragraphs, patentability is examined in terms of the types of patent protection available.

(a) *Countries granting "Product" patents.* Generally, no patent protection would be available in these countries if there has been a prior disclosure of the structure of the compound. The investigator making the prediction would be able to secure patent protection, but only if the patent application is filed prior to the appearance of the publication, and only if he describes how to prepare the compound and if he is able to demonstrate a utility for that compound. (In USA and Canada periods of one and two years, respectively, are permitted between appearance of a publication and filing of a patent application.)

(b) *Countries granting "Process" patents.* The requirements for the grant of a "Process" patent vary from one country to another. While in a few countries the act of prediction may have a minimal effect on subsequent patentability of a process, in many others, if the compound has been previously described, protection is available only if it is made by a "chemically inventive" process. In practice, most known chemical reactions are regarded as being "analogy" processes, so that where the compound has been pre-

viously described, no process protection would be available for any process which would be obvious to a skilled chemist.

(c) *Countries granting "Composition" patents.* If a specific biological activity is predicted it would be very difficult to obtain patent protection for a formulation unless the formulation was intended for use in a therapeutic area not anticipated by the predictor, and only if such use requires a type of formulation different from that used for the predicted purpose.

(d) *Countries granting "Method of Treatment" patents.* Patent protection would be available in these countries only if a therapeutic use, other than that predicted, had been discovered and if that use was not obvious over the predicted activity.

In summary, the patentability of compounds predicted to be biologically active would appear to be most seriously compromised in countries granting "Product" patents, and severe problems would be encountered also in countries which grant "Process", "Composition", and "Method of Treatment" patents.

Examination of Appendix C indicates that the majority of countries grant "Process" patents, although only a few grant "Product" patents. These are countries particularly prominent in drug development. Of further relevance is the circumstance that patent laws are constantly changing and on the horizon is the "European Patent" to be granted by the European Patent Convention, to which 21 European countries are expected to adhere. It is anticipated that this Patent will grant "Product" protection for novel drugs *per se*. "Product" patents are regarded in many quarters as one of the best types of patent protection available, and serve as an important incentive in the synthesis of potential new drugs. In the absence of this incentive it is likely that many structures, such as those shown in Appendix B, may never be synthesized and tested.

Conclusions and Recommendations

The aim of this report has been to focus the attention of medicinal chemists on some of the consequences that arise from the increasing level of sophistication with which structure activity relationships can now be analyzed. These analyses permit the prediction of allegedly biologically active compounds. If medicinal chemists were indeed able to develop useful therapeutic agents *via* such structure predictions, this would represent an advance of major proportions with widespread consequences. Whether or not the alleged biological activity is present, there is nevertheless a serious effect on patentability, because investigators who predict structures only infrequently also synthesize and test them, and the incentive for others to do so appears to be minimal, in large part because the possibility of obtaining patent protection is either lost or greatly diminished. The value of being able to predict structures with alleged biological activity appears therefore to be marginal at the present time, because of the adverse effect on patentability, and equally because they usually represent hypotheses that, for the reasons cited, are likely to remain forever untested.

In view of these considerations, the *ad hoc* Committee makes the following recommendations:

- (i) Medicinal chemists who publish predictions of allegedly active compounds should be urged to consider it their responsibility to synthesize and test such compounds or to arrange to have this done. "Predictions"

per se are of little practical value unless the underlying hypotheses are tested experimentally.

- (ii) Journal editors and editorial boards should consider the adoption of policies which discourage the publication of manuscripts containing "predictions" if they are not accompanied by the synthesis and testing of the predicted compounds.

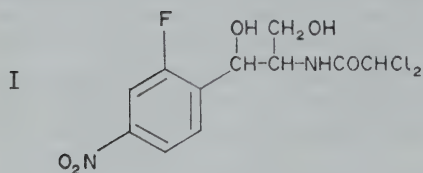
Appendix A

Recent Reviews on Quantitative Structure-Activity Relationships

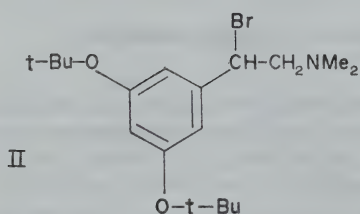
1. P. J. GOODFORD, 'Prediction of Pharmacological Activity by the Method of Physicochemical-Activity Relationships', in *Advances in Pharmacology and Chemotherapy* (S. GARATTINI, A. GOLDIN, F. HAWKINS and I. KOPIN, eds.), Volume II, pp. 52-99. Academic Press, New York, 1973.
2. A. VERLOOP, 'The Use of Linear Free Energy Parameters and Other Experimental Constants in Structure-Activity Studies', in *Drug Design* (E. J. ARIËNS, ed.), Volume III, pp. 133-187. Academic Press, New York, 1972.
3. C. HANSCH, 'Quantitative Structure-Activity Relationships in Drug Design', in *Drug Design* (E. J. ARIËNS, ed.), Volume I, pp. 271-342. Academic Press, New York, 1971.
4. M. S. TUTE, 'Principles and Practice of Hansch Analysis: A Guide to Structure-Activity Correlation for the Medicinal Chemist', in *Advances in Drug Research* (N. J. HARPER and A. B. SIMMONDS, eds.), Volume 6, pp. 2-77. Academic Press, New York, 1971.
5. J. W. MCFARLAND, 'On the Understanding of Drug Potency', in *Progress in Drug Research* (E. JUCKER, ed.), Volume 15, pp. 123-146. Birkhauser Verlag, Basel, 1971.
6. *Strategy of Drug Design* (W. P. PURCELL, G. E. BASS and J. M. CLAYTON, eds.). John Wiley and Sons, New York, 1973.

Appendix B

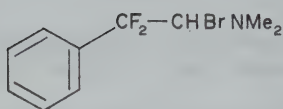
Some Predicted Structures Alleged to be Biologically Active



Predicted to possess better antibiotic activity than chloramphenicol, the corresponding des-fluoro derivative [*J. Amer. Chem. Soc.* **85**, 2817 (1963)]

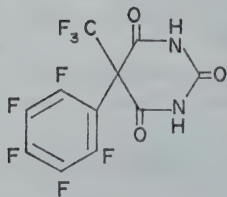


III

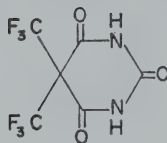


Predicted to be more active α -adrenergic blockers than known 2-bromo-2-phenylethylamines [*Biochem. Pharmacol.* **17**, 709 (1968)]

IV

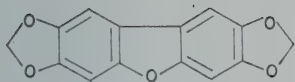


V

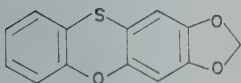


Predicted to be more potent hypnotics than currently available barbiturates [*J. Med. Chem.* **11**, 1 (1968)]

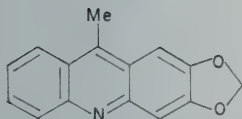
VI



VII

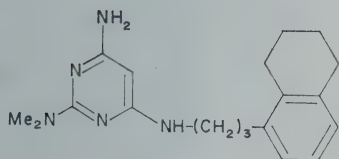


VIII



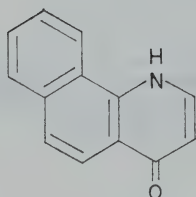
Predicted to be more potent than benzodioxole as a synergist of the pesticidal action of carbaryl [*J. Med. Chem.* **11**, 920 (1968)]

IX

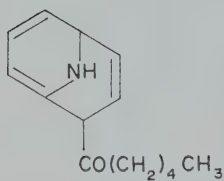


Predicted to be a more potent dihydrofolate reductase inhibitor than known tetrahydrofolate analogues [*J. Pharm. Sci.* **56**, 92 (1967)]

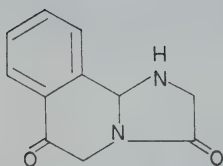
X



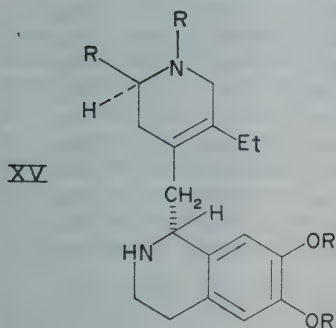
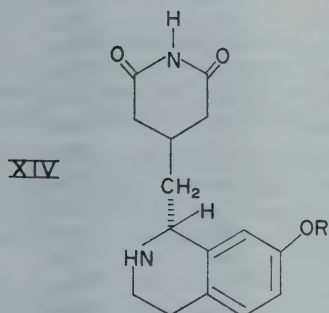
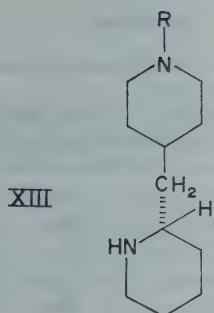
XI



XII



Predicted to be more potent antihypertensive agents than the benzothiadiazines [*Drug Design* (E. J. ARIENS, ed.) Volume I, p. 402. Academic Press, New York, 1971]



Predicted to be more potent protein synthesis inhibitors and amebicides than emetine or cycloheximide [*Proc. Nat. Acad. Sci.* **56**, 1867 (1966)]

Appendix C

Types of Patent Claim Allowed in Various Countries*

Country	Product	Process	Pharmaceutical composition	Method of treatment
Argentina	No	Yes	No	No
Australia	Yes	Yes	Yes	No
Austria	No	Yes	No	No
Belgium	Yes	Yes	Yes	Yes
Bulgaria	No	Yes	No	No
Canada	No	Yes	Yes	No
Chile	No	Yes	No	No
Columbia	No	Yes	No	No
Cuba	Yes	Yes	Yes	Yes
Czechoslovakia	No	Yes	No	No
Denmark	No	Yes	No	No
Federal Republic of Germany	Yes	Yes	Yes	No
Finland	No	Yes	No	No
France	Yes	Yes	Yes	No
German Democratic Republic	No	Yes	No	No
Hungary	No	Yes	No	No
India	No	Yes	No	Yes
Ireland	Yes	Yes	Yes	No
Israel	Yes	Yes	Yes	Yes
Italy	No	No	No	No
Japan	No	Yes	No	No
Mexico	No	Yes	No	No
Netherlands	No	Yes	No	No
New Zealand	Yes	Yes	Yes	No
Norway	No	Yes	No	No
Pakistan	No	Yes	Yes	No
Philippines	Yes	Yes	Yes	Yes
South Africa	Yes	Yes	Yes	Yes
Spain	No	Yes	No	No
Sweden	No	Yes	No	No
Switzerland	No	Yes	No	No
UK	Yes	Yes	Yes	No
USA	Yes	Yes	Yes	Yes
USSR	No	Yes	No	No
Venezuela	No	Yes	No	No
Yugoslavia	No	Yes	No	Yes

*BAXTER, *World Patent Law and Practice*, Vol. II. Matthew-Bender and Co. Inc., New York, 1973.

REPORTS OF IUPAC BODIES

SUB-COMMISSION ON PLASMA CHEMISTRY (I.2.1)*

Munich, 24-25 August 1973

Present: Dr. C. W. BECKETT (Chairman), Prof. M. FOEX, Dr. J. R. HOLLAHAN, Prof. E. MOLINARI, Prof. H. SUHR (Members); Prof. A. T. BELL, Dr. C. BONET (Observers).

1. The possibility of a change in status from Sub-Commission to Commission was considered from various points of view. It was decided to defer making any recommendation through the parent Commission (I.2: Thermodynamics and Thermochemistry) until the programmes of the Sub-Commission were developed more fully, probably by the 28th IUPAC Conference (1975).

2. A membership of twelve would be retained for the next biennium, but some changes were proposed in order to include Prof. BELL and Dr. BONET who had been active in the work of the Sub-Commission since 1971.† Prof. SUHR agreed to succeed Dr. BECKETT as Chairman.

3. An International Symposium on Plasma Chemistry had been organized by the Commission to take place in Kiel (6-10 September 1973) after the XXVII IUPAC Conference. Six invited papers and 52 contributed papers would be presented and an attendance of 200 was anticipated.

4. A subcommittee was formed to consider standards for measurement and calibration in the field of plasma chemistry: it was hoped to convene a meeting for discussions in 1974. A second subcommittee was established to review available data compilations which might be used in computations related to theoretical and design problems. This subcommittee would also assess what types of data were needed for the future. Another subcommittee was set up to determine guidelines for authors preparing papers for publication. A written report would be prepared, detailing the types of information which should be included and the desirable format for their publication. Yet a further subcommittee was created to assess the needs of industry with regard to plasma chemistry research. This group would report on the types of fundamental study which needed to be performed and the types of data which needed to be accumulated to aid industry.

5. A round table discussion on engineering applications of thermal plasmas related to heat and mass transfer between plasmas and condensed phases (with or without chemical reactions) was proposed for sponsorship by, but at no cost to IUPAC. This special meeting was provisionally scheduled for November 1975 at the CNRS laboratories in Odeillo, Font Romeu, the arrangements to be made by Prof. FOEX and Dr. BONET.

6. A general meeting, similar in character to the 1974 International Symposium on Plasma Chemistry in Kiel, was planned in Vienna for four days during October 1975. The main topics would be:

- (i) elementary chemical reactions in plasmas,

*See also *Comptes Rendus XXVII Conference: Part B*, page 117.

†See *Comptes Rendus XXVII Conference: Part A*, page 43.

- (ii) chemistry of gas-phase and gas-solid processes under plasma conditions,
- (iii) plasma chemical diagnostic techniques,
- (iv) inorganic and organic syntheses under plasma conditions.

A Programme Subcommittee was appointed, to include Prof. MOLINARI, Prof. SUHR, Prof. BELL, and Dr. BECKETT. Help in organizing the meeting had been offered by Prof. H. PERTELE (Technische Hochschule Wien). Cosponsorship with IUPAC by IAEA was being discussed, and it was possible that lecture facilities and other services might be provided by IAEA. It was decided to publish extended abstracts (1,000 words) and to sell these after the meeting for a price to be determined. A registration fee of \$50.00 was envisaged (inclusive of abstracts booklet).

7. The creation was discussed of a Bulletin to carry information about technical meetings, book reviews, notices of data collections, and other items of general interest to plasma chemistry researchers. Prof. BELL summarized possibilities for its preparation, printing, and distribution.

8. The Sub-Commission was currently preparing a comprehensive Bibliography of the plasma chemistry literature, the work being carried out under the direction of Prof. BELL. Some 4,000 references covering the period 1856-1970 had been contributed by Dr. D. J. SPEDDING (Auckland University, New Zealand) and another 143 references for 1971 by Dr. B. BLAUSTEIN (US Bureau of Mines). This material was now being sorted into six categories:

- (i) organic reactions,
- (ii) inorganic reactions,
- (iii) deposition of polymer films,
- (iv) deposition of inorganic films,
- (v) surface modification of solid materials,
- (vi) equipment design and operation.

Upon completion of the sorting, the references would be retyped in a form suitable for photooffset printing.

After the initial Bibliography was completed, it was intended to prepare annual supplements. Each supplement would contain the references to plasma chemical studies for one year plus a short abstract of the papers. The latter would greatly assist in improving the usefulness of the Bibliography. Preparation of the supplements would be carried out by either visual or computer scans of *Chemical Abstracts*. In addition, extensive use would be made of bibliographic lists prepared by individuals in a number of countries. It was anticipated that not only journal citations but also those of theses and government publications could be included.

Various mechanisms of issuing the Bibliography were considered. The favoured approach was to obtain publication funds from IUPAC for photooffset printing, distribution to be free of charge to some 300 active individuals in a Directory of Plasma Chemistry Research. The supplements would be sold at a small price to cover the costs of their printing and distribution.

H. SUHR

MACROMOLECULAR DIVISION WORKING PARTY ON MOLECULAR CHARACTERIZATION OF COMMERCIAL POLYMERS

Paris, 23 November 1973

Present: Dr. SCHOLTE (Chairman), Dr. ASSIOMA, Prof. BENOÎT, Dr. CROUZET, Dr. HOLMSTRÖM, Dr. KROZER, Dr. LEBRASSEUR, Dr. MULA, Dr. PANARIS, Dr. PEYROUSET, Dr. PRECHNER, Dr. ROTT, Dr. SERVOTTE, Dr. STRAZIELLE, Dr. VERSCHAVE, Dr. DE VRIES.

Meeting held at Brussels (17 November 1972)

A report on the deliberations had been published in *Information Bulletin* No. 45 (May 1973), pp. 50-53.

Molecular Characterization of Low Density Polyethylene Fractions

The meeting was devoted to this subject. The fractions from sample LDPE (IUPAC) had been prepared by Dr. PANARIS (SNPA, Lacq).

Fractionation of LDPE B Sample. Dr. PEYROUSET (SNPA) presented the method of fractionation. Fractionation was realized by preparative GPC with a set of six columns each containing spherosil: B(100 Å)—B/c—D—E—F and G ($\sim 10,000$ Å). 50 g of LDPE were dissolved in TCB at $C = 1\% + 1\%$ antioxidant. Each time, 100 ml of solution were fractionated at 150°C with a flow time of 50 ml/min in 19 fractions (volume of each fraction: 250 ml). Only the middle fractions (6, 7, 8, 10, 12, 14, and 16) were studied by the participants of the Working Party.

Intrinsic Viscosity Determinations. The intrinsic viscosities were determined mainly in TCB at 135°C except for two series.

(a) In decaline at 135°C and the $[\eta]$ values in TCB were calculated by using the relation $[\eta]_{\text{TCB}}^{135} = 0.9 [\eta]_{\text{dec}}^{135}$ [from the report of Dr. GLENZ (Hüls)].

(b) In *p*-xylene at 105°C , but $[\eta]$ in *p*-xylene at 105°C was practically identical to $[\eta]$ in TCB at 135°C [Dr. HOLMSTRÖM (Göteborg)].

Dr. SERVOTTE (Solvay, Brussels) gave also the $[\eta]\theta$ determined in diphenyl ether and the expansion coefficient

$$\alpha_{\eta}^3 = \frac{[\eta]_{135}^{\text{TCB}}}{[\eta]\theta}$$

α_{η}^3 increased from 1.4 for F_{16} to 1.9 for F_6 .

If one considered the results in TCB, the values were in relatively good agreement (except may be for two series). The divergence in $[\eta]$ values was about 10% and could not be explained by the experimental conditions. In order to explain this divergence, it would be necessary to plot all results $[\eta]_{\text{sp}}/c$ as a function of c in the same graph.

Osmometry and Light Scattering Determinations. There were only two series of values for M_n (number average molecular weight) and M_w (weight

average molecular weight) by using osmometry and light scattering. In these circumstances it was not possible to draw a definitive conclusion. The M_n values were in good agreement, but the M_w values by light scattering were not consistent. The difference between the two series was difficult to explain.

Results from Gel Permeation Chromatography. Firstly, the experimental procedures for GPC (calibration and method of correction for long branches) were described and discussed. The divergence in results was not very large and for each fraction the precision was about $\pm 20\%$.

Fraction	$(M_w^*)_{\text{aver.}} \cdot 10^{-3}$	$(M_w^{\text{corr}})_{\text{aver.}} \cdot 10^{-3}$
F ₆	232	441
F ₈	150	274
F ₁₀	101	170
F ₁₂	65	106
F ₁₄	40.4	63
F ₁₆	25.7	33.4

The differences in experimental methods (calibration, correction for long branching) were not the only source of discrepancy in the GPC results. For instance, the results obtained by workers using different methods did not show a systematic discrepancy for each fraction.

Future Programme

A forthcoming programme was decided. Dr. SERVOTTE and Dr. PANARIS accepted to deliver one unfractionated HDPE sample and unfractionated LDPE sample (LDPE B IUPAC sample) for molecular characterization. It was also decided that the next meeting would take place at the beginning of June 1974 at Strasbourg.

H. BENOÎT

IUPAC-IUB COMMISSION ON BIOCHEMICAL NOMENCLATURE (CBN)

Santiago de Compostela, 3-6 May 1974

Present: Prof. O. HOFFMANN-OSTENHOF (Chairman), Dr. W. E. COHN (Secretary), Dr. B. L. HORECKER, Prof. P. KARLSON, Prof. C. LIÉBECQ, Prof. E. C. WEBB. Dr. K. L. LOENING participated as an Observer from the IUPAC Commissions on Macromolecular Nomenclature (CMN) and on Nomenclature of Organic Chemistry (CNOC), Dr. R. DYBKAER as an Observer from the IUPAC Commission on Quantities and Units in Clinical Chemistry (CQUCC), and Prof. E. C. SLATER as an Observer from the IUB Commission of Editors of Biochemical Journals (CEBJ).

Minutes of Previous Meeting

The minutes of the meeting held at Meersburg on 20-23 June 1973 [see *Information Bulletin* No. 47 (March 1974), pp. 1-6] were approved.

Chairman's Report

HOFFMANN-OSTENHOF reported that 'Nomenclature of Corrinoids' would be published by IUPAC in August 1974 as Provisional Nomenclature Appendix No. 40 to the *Information Bulletin*. The revised version of 'Nomenclature of Cyclitols' was scheduled for publication in *Pure and Applied Chemistry* [37, 283 (1974)], as was that of 'Nomenclature of Quinones with Isoprenoid Side-chains' [38, 439 (1974)]. 'Nomenclature of Tocopherols and Related Compounds' was being prepared for publication by IUB in *Arch. Biochem. Biophys.* and it would be issued subsequently (in 1975) by IUPAC as a Provisional Nomenclature Appendix. 'Nomenclature of α -Amino Acids' had been approved by IUB, but not yet by IUPAC. Over 4,000 copies of *Enzyme Nomenclature Recommendations 1972** had been sold to date.

Previously Published Documents under Reconsideration:

- (i) 'Abbreviations and Symbols, 1965'. LIÉBECQ would replace DILLMANN as Convenor, with DILLMANN, COHN, and KLYNE as members of the redrafting subcommittee.
- (ii) 'Peptides'. A revision and expansion of Section 5 was under consideration.
- (iii) 'Miscellaneous Compounds' (Vitamins, Coenzymes). The vitamin A section should be revised and expanded, and be integrated into a second part of 'Carotenoids'. The vitamin K section needed attention. HOFFMANN-OSTENHOF would discuss these points with ISLER and devise a procedure. 'Calciferols' would be reviewed by KARLSON for possible revision. 'Flavins' was to be considered as an addition: a Convenor was needed for the submittee and HOFFMANN-OSTENHOF would seek a suitable person.
- (iv) 'Folic Acids' should be redrafted to concur further with the IUNS document on the subject. Pterins might be included. COHN was to prepare a draft document.
- (v) 'Carbohydrates-I' [Tentative Nomenclature Appendix No. 7 (September 1970) to *Inf. Bull.*]. This document should be revised by CBN and CNOC for publication as definitive rules as soon as a Convenor could be found for the subcommittee.
- (vi) 'Carotenoids' [Tentative Nomenclature Appendix No. 19 (February 1972) to *Inf. Bull.*]. A few late comments would be handled by KLYNE, who would then submit the final revised (and approved) document for publication in *Pure and Applied Chemistry*.
- (vii) 'Polypeptide Conformation' [*Pure and Applied Chemistry* 40(3) (1974), in press]. HOFFMANN-OSTENHOF was to consult KENDREW to ascertain if any revisions were necessary.
- (viii) 'Enzymes'. Annual minor revisions (corrections, etc.) to the 1972 Recommendations were contemplated, these to be published as normal CBN documents. Triennial supplements, as supplementary volumes collecting and integrating the preceding annual releases, were contemplated, with a completely new edition in the longer term (6-8 years). Advertisment of this procedure and calls for contributions from all workers and suppliers would be undertaken via CEBJ journals. Report

*Available from Elsevier Scientific Publishing Co., Amsterdam.

forms, costs of supplementary volumes, *etc.*, were discussed and were under active investigation. The deadline for receipt of material for the first annual revision statement was 31 December 1974 (in WEBB's hands). Several subcommittees to deal with Proteinases, Nucleases, Polymerases, Oxygenases, and Protein Biosynthesis Factors, were being set up.

Proteins

Consideration was given to the possibility of combining several CBN efforts to clarify and name members of protein families (*e.g.*, thrombin, plasmin, fibrinogen; collagens; histones; ribosomal proteins; enzyme proteins) into one enterprise, including such general matters as description of chains and homologies. HORECKER and KARLSON would prepare a draft statement of policy, procedure, and scope of the enterprise as a guide to specific action. 'Factors in Protein Biosynthesis'. A subcommittee would be established to recommend a uniform nomenclature in this area. HORECKER would seek a Convenor and recommend members.

Peptide Hormones

Final revisions and changes were presented by KARLSON (Convenor) and discussed. The revised document would be circulated once more and sent for approval by the respective authorities of IUB and IUPAC.

Catecholamines

There was a need for trivial names. HORECKER was to enlist a Convenor.

Phosphorus Compounds of Biological Importance

The draft formulated by COHN was discussed and the individual entries in the several tables were examined. COHN would redraft the tables and add these to the preamble, to be written by KLYNE. The document was to list systematic ('phosphate') names, inverted ('*O*-phosphono' and 'phospho') names, and symbolic representations for each entry; the list would be representative rather than exhaustive.

Lipids (revision and extension)

KARLSON (Convenor) reported on the present rather preliminary state of the considerations and the problems of trivial names (*e.g.*, globotriose, lactotriose). HIRSCHMANN (Convenor for the original Lipid document), SNYDER, STOFFEL, VEIBEL, and VÖGTLE, had joined WEIGANDT in the subcommittee. WEIGANDT and HIRSCHMANN would be particularly concerned with glycosphingolipids. All interim reports of the group would be circulated to CBN by the Convenor.

Lipoproteins

CEBJ had asked CBN to undertake some effort in this area (of HLP, VHLP, VLLP, apo-LP, *etc.*). HORECKER and KARLSON would seek interested persons to form a subcommittee.

Enzyme Units

The present chapter in *Enzyme Nomenclature Recommendations 1972* and 26

a proposed redraft by COHN and DYBKAER were discussed at length. Various proposals were made and criticized. LIÉBECQ would draft a new version for circulation to CBN (and CEBJ), with the aim of creating a separate CBN document for immediate publication as well as a revised Chapter 4 for this book.

Immobilized Enzymes

No report had been received from the subcommittee.

Interconvertible Enzymes

HORECKER reported on a first draft by HOLZER, which had been circulated to a number of workers and had elicited a number of comments. New terms introduced were 'allozymes' (polymorphs of allelic origin), 'metazyme' (epigenetic modification), and symbols 'o' (ortho, for original) and 'm' (meta, for modified). Discussion led to the conclusion that this effort should be integrated with work on Multiple Forms of Enzymes, published separately in 1973, and in *Enzyme Nomenclature Recommendations 1972*, and form a revised Chapter 3 in the latter. HORECKER would produce a new draft for consideration by HOLZER and KARLSON, and later by CBN.

Cytochromes

A letter from KAMEN (Convenor) indicated that work was in progress. SLATER was to communicate to KAMEN certain principles that CBN wished to see incorporated.

Polynucleotide Conformation

The discussion of this document among SUNDARALINGAM (originator), CRAMER (Convenor), and RAMACHANDRAN was being correlated by KLYNE.

Carbohydrates

- (i) 'Monosaccharide Conformations'. Some criticisms had been circulated to the subcommittee by COHN. These had been referred to KLYNE for resolution and the preparation of a new draft.
- (ii) 'Polysaccharide Nomenclature'. Although no document was formally before CBN, a draft proposal had been criticized on the grounds that present polymer nomenclature could adequately fulfill the need. A draft indicating this, prepared by COHN, with the aid of FOX (CMN) and TIPSON (Anglo-American Carbohydrate Nomenclature Committee, and member of the CNOC-CBN subcommittee) was preferred by CBN and had been referred to the subcommittee.
- (iii) 'Polysaccharide Conformation'. A draft from MARCHESSAULT's subcommittee had been circulated to CBN. Efforts were being directed to ensure conformity with the previous Polypeptide document (KLYNE) and an emerging general conformation document (CORRADINI of CMN).
- (iv) 'Oligosaccharide Nomenclature'. A document from the British Carbohydrate Nomenclature Committee had been circulated by CROSS (CNOC and CMN), but it was not formally before CBN or the subcommittee. COHN had made some suggestions to bring this into line with existing symbolism.

Tetrapyrroles

A fourth draft by BONNETT's subcommittee was distributed at the meeting, and was now formally before CBN and CNOC. Some criticisms (by SLATER of the cytochrome part, by COHN of the abbreviations) were made. All criticisms would be referred back to BONNETT by HOFFMANN-OSTENHOF. CNOC would consider the document at its meeting in UK later in the year.

Prostaglandins

The CNOC-CBN subcommittee comprised KARLSON (Convenor), HORTON (Edinburgh), MARTEL (Romainville), BERGSTROM (Stockholm), and HOFFMANN-OSTENHOF. The Organic Nomenclature Committee of the American Chemical Society in considering the Nelson report, had written a good analysis of it, and had turned this analysis and its interest in the matter over to the CNOC-CBN subcommittee. The objectives of the latter were (1) systematic organic nomenclature, and (2) trivial names informative as to structure.

Natural Products

The purpose of the present CNOC document was to create nomenclature guidelines for discoverers and to standardize semisystematic nomenclature in areas already explored but lacking semisystematic nomenclature. CBN was interested in a biochemically-oriented document, but proteins might dominate CBN's interests.

Isotopically-labelled Compounds

CBN reiterated its desire to be consulted in the formulation of this document, because of the predominating concern of biochemists and the previously adopted system of CEBJ. Although not members of the subcommittee, COHN and DERMER had made detailed criticisms of certain principles embodied in the present CNOC drafts. These principles were described to CBN by COHN. HOFFMANN-OSTENHOF would convey CBN's concern to CNOC.

Stereochemistry of Macromolecules

The Commission on Macromolecular Nomenclature was currently constructing a document dealing with the stereochemistry of macromolecules. This work was being integrated with past and present enterprises on conformation (polypeptides, polysaccharides, polynucleotides) to the greatest extent possible.

Publication of CBN Documents by IUB

CEBJ would henceforth ask only one biochemical journal, instead of two, to set type and print CBN documents. Other journals, as at present, would be free to reprint by photo processes.

Membership of CBN

Terms of office of IUB members of CBN might be specified in the future. The terms of IUPAC members were governed by draft Standing Orders of the IUPAC Executive Committee regarding CBN, which had been approved by HOFFMANN-OSTENHOF, COHN, and KLYNE.

As a replacement for WHELAN, who had resigned, W. B. JAKOBY (National Institutes of Health, USA) was unanimously recommended to IUB.

Date and Place of Next Meeting

CBN desired to meet jointly with CEBJ in UK in June or July 1975.

W. E. COHN

MACROMOLECULAR DIVISION WORKING PARTY ON SUPPORTED POLYMER FILMS (WSPF)

Garmisch, 15 May 1974

Present: Mr. P. H. FINK-JENSEN (Chairman), Dr. U. ZORLL (Secretary), Mr. G. CHRISTENSEN, Prof. K. HAMANN, Dr. K. M. OESTERLE, Prof. D. PAGANI, Dr. J. PETIT, Mr. H. K. RAASCHOU-NIELSEN, Dr. H. SPOOR, Mr. A. TOUSSAINT, Dr. D. WAPLER. Attending as guests were H. L. GERHART (FSPT) and L. PORTIN (SLF).

Minutes of Previous Meeting

The minutes of the meeting held at Munich on 23-26 August 1973 had been published in *Comptes Rendus XXVII Conference: Part B*, pp. 327-333.

Report of Chairman

Mr. FINK-JENSEN reported on the activities since the previous meeting, including correspondence with the FSPT Liaison Committee. He told members that further reprints of 'Recommended Methods for the Analysis of Alkyd Resins' [*Pure Appl. Chem.* **33**, 411 (1973)] had been made and were now on sale at the IUPAC Secretariat.

In response to a request from ISO, that an information gap was felt to exist between WSPF and that organization's technical committees concerned with the paint field, Mr. FINK-JENSEN informed the group that Mr. RAASCHOU-NIELSEN and Dr. L. A. O'NEILL had been nominated as IUPAC representatives in the ISO committees TC 35/SC 9 and 10. The advantage of this arrangement had already been felt during The Hague session of ISO earlier this year, where the standpoint of WSPF with respect to saponification values could be formulated during the meeting of ISO/TC 35/SC 10.

Reports from Project Leaders

The Chairman indicated on behalf of Dr. O'NEILL that the report on analytical methods for alkyd resins had already been reviewed in individual journals such as *Verfkroniek* and *Färg och Lack*. The corresponding results on analysis of acrylic resins had been sent for publication in the *Journal of Paint Technology*. Similar work on polyurethanes was finished and a paper about it was being prepared. Finally, work on analytical methods for polyamide resins was proceeding as scheduled.

Mr. RAASCHOU-NIELSEN reported that the task group on information retrieval had continued its efforts to give the survey a broad international basis, particularly with respect to the literature available in USSR. Contact with pertinent colleagues in that country was being taken into consideration.

The programme of work in the adhesion group was to be redefined, according to Dr. ZORLL, who had taken over responsibility from Dr. J. A. W. VAN LAAR. Because progress had been made in the field of systems for adhesion measurement, the aspects of new instruments and their range of performance should be included in the work to be done.

It was reported by Prof. HAMANN that in the group for postgraduate educational studies various possibilities were being discussed with regard to versatility and suitability of that form of professional training.

Unfortunately, Mr. A. R. H. TAWN could not be present to report on the new activities regarding solvent media interaction.

New Members

Various members proposed to name some new colleagues of the younger generation to become cooperators for WSPPF, particularly those in laboratories of industry and institutes who would be in a position to carry out tasks given the group as such in the future. A suggestion had been made by Prof. C. G. OVERBERGER that a member of the ACS Division of Organic Coatings and Plastics Chemistry should join WSPPF. Prof. R. MYERS had been proposed and the group expressed full satisfaction with that nomination. There was general agreement with the suggestion of the Chairman, that a representative from each of the four federations should be invited to become a member of WSPPF.

International Cooperation

On behalf of FSPT, Dr. GERHART reported on extensive efforts to improve international cooperation. In the framework of this action, the existing associations should also be linked in a suitable way with WSPPF.

Common international efforts should be based on the ICCCI-organization, about which the group was already informed. The field of action could comprise such topical problems as environmental protection and controls for toxic materials. Much of that work could be carried out by mail so that there was virtually no dependance on regular meetings.

With the exception of FATIPEC, where a final point of view had not yet been attained, other associations had expressed their readiness to co-operate in the sense mentioned.

Date and Place of Next Meeting

The original plan to hold the next meeting in Madrid in September 1974 was not now felt to be feasible. Consequently, it was proposed to meet in Brussels in November 1974.

U. ZORLL

MACROMOLECULAR DIVISION WORKING PARTY ON MOLECULAR CHARACTERIZATION OF COMMERCIAL POLYMERS

Strasbourg, 28 June 1974

Present: Dr. BALL (Chairman), Dr. ASSIOMA, Prof. BENOÎT, Dr. GALLOT, Dr. HOLMSTRÖM, Dr. LECAT, Dr. PRECHNER, Dr. ROTT, Dr. SCHOLTE, Dr. SERVOTTE, Dr. STRAZIELLE.

Meeting held at Paris (23 November 1973)

A report on the deliberations had been published in *Information Bulletin* No. 49 (March 1975), pp. 23-24.

Molecular Characterization of Fractionated Low Density Polyethylene

The problem of characterization of fractions from sample LDPE B (LDPE IUPAC) was reexamined (see report of previous meeting). Some further results were presented by Dr. SCHOLTE (Solvay, Brussels—light scattering, ultracentrifugation, GPC) and by Dr. BALL (BASF, Ludwigshafen—osmometry, light scattering, GPC). After announcing the new values for the intrinsic viscosity $[\eta]$ and weight average molecular weight (M_w), the results were examined and discussed.

Molecular Characterization of Unfractionated Polyethylene

Consideration was given to the results obtained from the recent programme on the two unfractionated polymers (rehomogenized), HDPE Eltex 6009 and LDPE B.

It was decided to present a paper, giving an analysis of the whole of the results of the Working Party during 1971-1974, at the International Symposium on Macromolecules (Madrid, 15-20 September 1974).

Future Programme

The future programme of study for the Working Party was agreed to be a determination of the molecular parameters and ramifications of the homogenized sample LDPE C. Persons interested in taking part in this study should contact Dr. STRAZIELLE (Centre de Recherches sur les Macromolécules, Strasbourg). The next meeting was scheduled for 17 January 1975 at Geelen.

H. BENOÎT

COMMISSION ON NOMENCLATURE OF ORGANIC CHEMISTRY (CNOC)

Dorking, 13-20 July 1974

Present: Prof. N. LOZAC'H (Chairman), Mr. S. P. KLESNEY (Secretary), Dr. K. BLÁHA, Dr. L. C. CROSS, Dr. H. GRÜNEWALD, Prof. W. KLYNE, Dr. K. L. LOENING, Prof. J. RIGAUDY (Titular Members); Dr. K. HIRAYAMA, Prof. S. VEIBEL, Prof. F. VÖGTLE (Associate Members); Prof. O. HOFFMANN-OSTENHOF [Observer, IUPAC-IUB Commission on Biochemical Nomenclature (CBN)]; Prof. J. CHATT [Observer, Commission on Nomenclature of Inorganic Chemistry (CNIC)]; Dr. D. C. VEAL [Observer, Interdivisional Committee on Machine Documentation in the Chemical Field (IDCMD)].

Minutes of Previous Meeting

The minutes of the meeting held at Würzburg on 15-22 August 1973 had been published in *Information Bulletin* No. 47 (March 1974), pp. 6-8.

Revision of Sections A, B, C, and D*

After consideration of its assignment on the revision and simplification of Sections A, B, C, and D, the working party (GRÜNEWALD, CROSS, and LOENING) concluded that in order to complete the task in an acceptable length of time it would be necessary to obtain additional help. It was estimated that the job might require the fulltime services of one person for about one year. In this connection, Dr. GRÜNEWALD had made enquiries to officials of Gesellschaft Deutscher Chemiker, the Chemical Society in UK, and the American Chemical Society, with the result that each Society had agreed tentatively to finance one-third of the cost on the condition that IUPAC would reimburse the monies when any profits were realized from the sale of the eventual publication. The person doing this work would be completely under the supervision of the working party, which in turn would report periodically to CNOC. It was agreed that the Chairman should send an official letter to the Bureau requesting the appointment of a person agreeable to all the relevant groups.

Section D: Rules for Organometallic Chemistry

There was an extended discussion on the recently published tentative version of Section D, in which Prof. CHATT participated on behalf of CNIC. In particular, a number of comments received on the document were considered and agreement reached on modifications of the text that were necessary, some points were referred for the advice of CNIC, and some further actions were specified for CNOC.

Section E: Fundamental Stereochemistry

Prof. KLYNE reported that he and Dr. CROSS had taken into account the decisions made at the previous meeting concerning the tentative version of Section E [*Information Bulletin* No. 35 (June 1969), pp. 36-80]. Dr. CROSS was preparing a revised document for publication in *Pure and Applied Chemistry*. It would now be necessary to list the items for Part II of Section E.

Section F: Natural Products and Related Compounds

The latest draft was examined and approved in principle. A number of minor corrections were listed and would be taken into account by Dr. CROSS and Prof. KLYNE. The amended document was to be circulated to CNOC and CBN, allowing 30 days for submission of comments. Thereafter, the document should be ready for publication as a Provisional Nomenclature Appendix to the *Information Bulletin*.

Cyclophanes and Polycyclic Arrays of Carbon Atoms

No criticism having been received of the draft on polycyclic arrays, it was accepted by CNOC subject to a slight modification. It was agreed that the working party (LOZAC'H, HIRAYAMA, LOENING, VÖGTLE, KAUFFMANN, ECKROTH) would finalize this document, dealing with the generalization of the Von Baeyer system, for distribution as a Provisional Nomenclature Appendix as proposals for study and solicitation of criticism.

**Nomenclature of Organic Chemistry*, 1971 (combined Sections A, B, and C); Section D: Tentative Nomenclature Appendix No. 31 to *Information Bulletin*, August 1973.

Discussion of a draft on phane nomenclature prepared by Prof. VÖGTLE, brought out a number of points. Consideration was given especially to nodal nomenclature and 'collapsing'.

Isotopically Modified Compounds

The revised draft nomenclature document of Prof. RIGAUDY was examined critically and the approved changes would be incorporated into a new document for further consideration by CNOC.

Anions, Cations, and Radical Names

It was agreed that this topic was large enough in scope to require a separate working party, for which the membership would be LOZAC'H (Convenor), RIGAUDY, TRAYNHAM, POWELL, GARST, GRÜNEWALD, SMITH.

Typographical Conventions

The meeting decided that typographical conventions should be made part of nomenclature recommendations. Where possible, the use of punctuation marks (.,; etc.) should have the same meaning and be used in the same way in all languages. It was emphasized that, at the minimum, uniformity should exist in English language usage in chemical nomenclature (e.g., 2-hexene vs hex-2-ene). The use of italics in printing atomic symbols in names was discussed. It was agreed that this question should be studied in a broader context, including other italicized terms, such as *cyclo*, *homo*, *seco*, etc. Ordering of letter and numerical locants in a name should also be considered.

Biochemical Nomenclature

Prof. HOFFMANN-OSTENHOF (Chairman of CBN) participated in discussions with CNOC on topics of mutual interest. He expressed satisfaction with the good cooperation between CBN and CNOC and he hoped this would continue. He reported that there was now a subcommittee on flavins and on vitamin D and that the document on folic acids was being revised. Other topics discussed were:

Lipids. Work was now under way. A document on glycolipids had been received by LOZAC'H. CNOC contact person for this subcommittee was VÖGTLE.

Lignins. A document on lignin nomenclature was partly written. CNOC contact person for the lignin working party was CROSS.

Prostaglandins. Dr. DERMER had sent a document entitled 'Systematic Nomenclature of Prostaglandins: Historical Review and Commentary' to Prof. KARLSON of CBN. CNOC contact for this working party was BLAHA.

Tetrapyrroles. A document on the nomenclature of tetrapyrroles was received by the joint CNOC-CBN subcommittee earlier in 1974. CNOC would study this document, its contact person being LOENING.

Carbohydrates. Prof. HOFFMANN-OSTENHOF briefly reviewed the history of recent carbohydrate nomenclature. He mentioned that WHELAN had withdrawn from this subcommittee, partly due to other commitments. CNOC contact person was CROSS. After long consultations in pursuance of previous deliberations, Prof. RIGAUDY proposed as a member of the subcommittee Prof. L. MESTER. Prof. HOFFMANN-OSTENHOF agreed with this proposal.

Amino Acids. A document approved by both CNOC and CBN was ready for publication. A short paragraph on the use of *homo* in amino acids should be added to this document. CNOC contact person was VEIBEL.

Cyclitols. A revised version of the tentative document on naming cyclitols was scheduled for publication in *Pure and Applied Chemistry* [37, 283 (1974)].

Carotenoids. Prof. KLYNE distributed to CNOC copies of a list of amendments to the document on 'Nomenclature of Carotenoids'. It was agreed that KLYNE should incorporate the agreed amendments and send the revised document for publication in *Pure and Applied Chemistry*.

Liaison with CNIC

CROSS was delegated to serve as the CNOC representative to the Inorganic Nomenclature Commission meeting later in 1974. He was asked to transmit the CNOC opinion that locant designations for ligands or substituents should be independent of chirality. Also, the use of lines, arrows, and dotted lines in formulae to indicate bonds or the edges of geometric figures varied in Section D. CNOC requested the advice of CNIC on how it wished formulae to be written in Section D.

Membership

It was agreed that new Members were needed to expedite and make more effective the work of the Commission and its working parties. In this connection the Chairman would propose Dr. W. H. POWELL (USA) as an Associate Member. CROSS would suggest a suitable person from the Chemical Society in UK, and KLYNE would propose a man from F. Hoffman-La Roche Co.

Interdivisional Committee on Machine Documentation in the Chemical Field

Dr. VEAL, Secretary of this Committee, participated in discussions on the future development of nomenclature and its relationship to machine documentation. He commented that it seemed desirable that the present Nomenclature Commissions of IUPAC should carry on their work as in the past but, in addition, an opportunity should be given to the Machine Documentation Committee to review and make suggestions where problems were seen.

Date and Place of Next Meeting

Dr. LOENING was to make initial contacts on a suitable meeting place in Spain and advise the Chairman accordingly. The period 24-31 August 1975 was tentatively agreed for the meeting.

S. P. KLESNEY

COMMISSION ON ELECTROANALYTICAL CHEMISTRY (V.5)

Jülich, 22-24 July 1974

Present: Prof. L. MEITES (Acting Chairman), Prof. E. BISHOP, Prof. Z. GALUS, Prof. H. W. NÜRNBERG, Prof. P. ZUMAN (Titular Members); Prof. J. JORDAN (Associate Member). The meeting was an interim one, with limited attendance from Commission Members, in order to progress selected nomenclature matters before the 28th IUPAC Conference (Madrid, 1975).

Classification and Nomenclature of Electroanalytical Techniques

Comments had been received from a wide circle of electroanalytical chemists and electrochemists to the proposals in Tentative Nomenclature Appendix No. 30 (August 1973) to the *Information Bulletin*. Careful consideration was given to all comments, except for those involving creation of new terms, and appropriate changes to the tentative document were approved. The amended document would be submitted via the Officers of the Commission for approval by the Analytical Chemistry Division Committee and publication in *Pure and Applied Chemistry*.

Sign Convention

Prof. MEITES was instructed to take into consideration the discussion of the meeting and to finalize the document on 'Recommendations for Sign Conventions and Plotting of Electrochemical Data'. The latter should then be submitted for publication as a Provisional Nomenclature Appendix to the *Information Bulletin*.

Terms and Symbols

Prof. BISHOP would try and arrange for all persons present to receive a reprint of the recently published recommendations of the Commission on Electrochemistry (I.3) on 'Electrochemical Nomenclature' [*Pure Appl. Chem.* 37, 499 (1974)]. This would ensure a minimum of overlap with the proposals being prepared on electroanalytical terms and symbols by Commission V.5.

After discussion it was agreed by those present at the meeting that the use of symbols λ and Λ , which had been used to denote equivalent conductance in the past to denote molar conductances in the future, was unacceptable. The Secretary of Commission V.5 would be requested to contact Commission I.3 in the hope that agreement could be reached on acceptable symbols for molar conductance and molar ionic conductance. The use of U and E_{ecm} should be discussed with Dr. PARSONS of Commission I.3. The use of symbols t_p for pulse duration, t_m for sampling time, and t_r for reversal of voltage ramp, ω for angular frequency, were considered. The symbol i_s was recommended for summit current, which was defined as the value of the current at an extremum (usually a maximum) on a plot of current against applied emf obtained either by the use of a small amplitude periodic excitation signal or by differentiation. The revised version of the proposed list of terms and symbols would be circulated to those present for further comment after the meeting.

P. ZUMAN

SECTION ON FOOD (VI.1)

Warsaw, 25-27 July 1974

Present: Dr. R. MARCUSE (Chairman), Dr. H. GUTHENBERG (Secretary), Dr. E. O. HAENNI, Dr. K. KOJIMA, Prof. M. NIKONOROW, Dr. K. OHNO, Mr. M. V. TRACEY, Dr. A. E. WASSERMAN (Titular Members); Dr. H. FISCHBACH, Dr. P. L. SCHULLER (Associate Members). The Food Section met at Warsaw in conjunction with the Commissions on Food Additives

and on Food Contaminants and some Members of the respective IUPAC bodies sat in as Observers at the other meetings.

Minutes of Previous Meeting

The minutes of the meeting held at Munich on 23-26 August 1973 had been published in *Comptes Rendus XXVII Conference; Part B*, pp. 219-223.

Chairman's Report

Dr. MARCUSE reported on the following activities:

- (i) The joint IUPAC-IUFoST Round Table discussion on Purity Requirements for Food Additives (29-31 August 1973, Hamburg). The contributions and comments had been published and distributed to the participants.
- (ii) The Joint FAO-WHO Conference on Food Additives and Contaminants (22-26 October 1973, Geneva). Two reports, one a general and the other a special one, were distributed to Members.
- (iii) Meeting of Coordinating Committee for Analytical Methods [6 April 1974, Oxford: see also *Inf. Bull.* No. 48 (October 1974), pp. 29-33].
- (iv) Discussion of the programme of the Food Section and particularly on the preparations of the IUPAC-IUFoST Working Party attended by US Members of the Section and its Chairman (17 May 1974, Washington, DC).
- (v) Meeting of the joint FAO-WHO Expert Committee on Food Additives (4-13 April 1974, Rome).
- (vi) Joint IUPAC-IUFoST Working Party on Critical Examination of Purity Criteria of Food Additives (29 July 1974, The Hague).
- (vii) Preparations for planned diversification of the programme of the Section.
- (viii) Elaboration of rules for the running of the Section as well as of guidelines for the Section Committee.
- (ix) Correspondence concerning
 - guidelines for single cell protein (SCP)
 - quality appraisal for meat and fish
 - PAG Working Group on Protein Methods for Cereal Breeders
 - single kernel analysis (Dr. HULSE, Ottawa)
 - collaborative minicolumn screening test for aflatoxins (Mr. ROMER, Washington)
- (x) Commitments of Members of the Section Committee as shown in the circular letter of 3 May 1974 to Members of the Committee.

Also, the Chairmen of the two Commissions attached to the Section reported on their activities by referring to distributed reports and adding certain comments.

Abolition of Sections

A recent circular letter from the IUPAC Secretariat on revision of the IUPAC Statutes and Bylaws and a proposal for abolishing Sections, was discussed. According to the proposal only the two Commissions attached to the Food Section would be maintained. However, according to information received,

the scope of the Food Section was expected not to be altered considerably.

Taking into consideration previous discussions concerning diversification of the programme, it was proposed that the two Commissions should be devoted to (a) food safety, and (b) food quality. It was presumed that the work of the two Commissions would be administered by a coordinating committee, which could be called Coordinating Committee on Food Chemistry, which might be given similar tasks as had been planned for the Food Section Committee. Special *ad hoc* groups might be delegated for specific items, such as natural toxicants (mycotoxins) or food additives. The Chairman informed Members of contacts with other Sections within the Applied Chemistry Division, mainly the Section on Pesticides, the Section on Oils and Fats, and the Section on Fermentation. Also, he referred to his personal initiative with regard to linguistic difficulties at meetings. His letter to the IUPAC Secretariat had been discussed at a meeting of the Executive Committee, which had agreed upon certain measures to be taken. Members gave their full support and agreed that further measures should be envisaged in order to make the action effective.

IUPAC-CEE Contract

The Chairman reported on the liaison with the Commission on Analytical Reactions and Reagents (V.1), mainly referring to the CEE commitment. A new scheme for selection of methods had been elaborated at the XXVII IUPAC Conference in Munich. Ten methods were to be delivered to CEE under the 1974 contract, of which seven methods had already been distributed for comment. A report had been prepared on the comments received.

Cooperation with International Agencies

The Chairman and some Members reported on contacts with various international agencies throughout the past working year:

- (i) By Chairman: Correspondence with Mr. G. Vos, Commission of the European Communities

- Letter from IUPAC Secretariat on FAO-WHO Expert Committee on Food Additives (revised specifications for five groups of additives)

- Correspondence with Dr. M. MILNER (PAG) in respect of the Working Group on Protein Methods for Cereal Breeders

- Correspondence with Dr. HULSE (PAG) in respect of micromethods to determine protein nitrogen and lysine nitrogen in very small samples (single seed analysis)

- Programme for the ICC Meeting (Vienna, May 1974) on analysis of SCP

- Information from ISO on some recently received methods

- Letter from Conseil d'Europe, offering collaboration

- Letter from European Food Emulsifier Manufacturers Association (EFEMA) offering collaboration.

- (ii) By Dr. E. SOMERS and Dr. KOJIMA: Contacts of Dr. R. MALIK (FAO) with some Members of the Section in order to prepare a meeting in October on an internationally coordinated food contamination monitoring programme. Members invited were asked to work not only on problems of analysis, but also on wider aspects of the project.

- (iii) By Mr. E. A. WALKER: Comments on aflatoxin sample series.

Guidelines for Running the Section

A draft of guidelines for running the Section as well as notes on the scope and the functions of the Food Section Committee had been distributed to Members. These guidelines included the introduction of project and membership sheets. It was agreed that a group of three Members (HAENNI, KOJIMA, MARCUSE) should discuss and further elaborate these guidelines and distribute revised drafts to all Members.

Diversification of Programme

The Chairman outlined what had happened with respect to the plans for diversification of the programme of the Applied Chemistry Division and the Food Section and mentioned particularly statements by Dr. H. EGAN during the XXVII IUPAC Conference (Munich, 1973) and a recent memorandum by Dr. A. F. LANGLYKKE. Several proposals had been received from Members. A memorandum elaborated by the Chairman had been distributed to Members on 24 June 1974. It was agreed that a group of three Members (HAENNI, KOJIMA, MARCUSE) should discuss this item by correspondence and elaborate proposals for distribution to all Members.

The programme of the Food Section was composed of those of its two Commissions, together with additional projects sponsored by the Food Section Committee. Members of the Section Committee would cooperate in the development of guidelines for running of the Section and in diversification of the programme, and also in elaborating plans for future symposia. Collaboration was particularly desirable for the development of the programme on food quality. As an example of and a basis for such a collaborative programme, Dr. WASSERMAN had elaborated a paper on Quality Factors for Meat. Dr. OHNO agreed to work with Dr. WASSERMAN in pursuance of this subject.

Attention would be given to matters arising from the minutes of the 1973 meeting in Munich. Items such as analysis of SCP and determination of cadmium were, for example, included in the Food Contaminants Commission programme, while benzo(a)pyrene and nitrosamines were part of that of the Food Additives Commission.

Certain items would be treated in collaboration with other IUPAC bodies:

- SCP analysis: together with the Fermentation Section (particularly determination of available lysine, purines, nucleic acids, S-amino acids)
- Antioxidants and mycotoxins: together with the Oils and Fats Section
- Heavy metals: together with the Pesticides Section
- Harmonization of collaborative studies: together with the Analytical Chemistry Division

Symposia

Members agreed that, as a principle, it would be desirable to arrange symposia in connection with annual meetings of the Section, particularly annual meetings between IUPAC Conferences. The Chairman repeated his earlier proposal to start a series on so-called Rapid Methods. Members agreed on the desirability of such symposia. It might, however, be difficult to implement this idea already in 1975. It was left to the Chairman to examine further the possibilities and, particularly, the interest of the local organizers of the 28th IUPAC Conference in Madrid. It might be suitable to plan only a limited

meeting for 1975, may be a seminar, which could serve as a test meeting for future symposia.

Dr. A. D. CAMPBELL suggested that industrial companies producing Rapid Methods-instruments should be invited to present proposals. According to Dr. HAENNI, people from industries using such instruments should report on their experiences. Mr. WALKER recommended that the Analytical Chemistry Division should be invited to participate. Dr. CAMPBELL, Dr. KOJIMA, Dr. W. KRÖNERT, and Dr. SCHULLER agreed to collaborate with Dr. MARCUSE concerning this subject.

For 1976 a Third Symposium on Mycotoxins was planned. Dr. M. JEMMALI would be interested to hold it in or near Paris. Further, Prof. A. RUTKOWSKI informed Members of his plan to organize a symposium on Smoked Foods, possibly as a joint IUPAC-IUFoST symposium, sponsored by the Polish Academy of Sciences and supported by the US Food and Drug Administration. It was intended to cover, among other items, analytical and technological questions.

A proposal had been made by Prof. WOLFF (US Drug Administration, Philadelphia), to arrange a symposium on Natural Toxicants. Dr. HAENNI reminded the meeting of his earlier proposal to organize a symposium on Drug Residues from Animal Feed in Food.

Membership

The Chairman informed members of the resignations of Dr. N. R. JONES (Titular Member) and Dr. D. N. RHODES (National Representative).

It was proposed that the following changes in membership assignments be made: from the Food Section Committee to the Commission on Food Contaminants—Prof. NIKONOROW and TRUHAUT, and Mr. TRACEY; from the Food Section Committee to the Commission on Food Additives—Dr. FISCHBACH and Dr. BERGSTRØM-NIELSEN; from the Commission on Food Additives to the Food Section Committee—Dr. EDHBORG. The Members who were present agreed. In the cases of Prof. TRUHAUT, Dr. BERGSTRØM-NIELSEN, and Dr. EDHBORG, the changes were subject to their concurrence.

Reports from Commissions

The report from the Food Contaminants Commission commented particularly on the future role of SCP in the Food Section programme. Members agreed that in spite of the fact that SCP for the time being was mainly of interest for feeding purposes, it was to be kept in the programme of the Commission. It was further agreed that Dr. J. D. LITTLEHAILES should be asked for advice.

Members also discussed the results of the collaborative study carried out by Dr. GUTHENBURG in collaboration with Dr. SCHULLER on the determination of mercury.

Various opinions were expressed concerning the requirements to be fulfilled by an IUPAC-recommended method and the further handling of the item. It was agreed to have Dr. GUTHENBERG's report distributed to Members for final comment.

Publications

The following publications were in process of being finalized:

- (i) By IARC as a joint project with IUPAC: Manual of Interim Methods with Test Results for Volatile Nitrosamines in Meat

- (ii) Supplement to 'Survey of Analytical Methods Available for the Estimation of Some Food Additives in Food' (*Pure Appl. Chem.* **26**, 75 [1971])—Estimation of Antioxidants
- (iii) Survey of Methods for Artificial Sweeteners in Food
- (iv) Determination of Mercury in Food
- (v) Cadmium in Food: Review of Available Methods
- (vi) A compilation of contributions to a panel discussion on Purity Requirements for Food Additives and Their Control (Hamburg, August 1973) was available
- (vii) Papers presented at the Second IUPAC Symposium on Mycotoxins in Food (Puławy, July 1974) would be published by Prof. JUSZKIEWICZ
- (viii) A report by Dr. WASSERMAN on Quality Factors for Meat would be distributed to Members for comment with respect to publication

Date and Place of Next Meeting

This would be during the 28th IUPAC Conference in Madrid. The Food Section and its Commissions would meet provisionally during 3-6 September 1975.

R. MARCUSE

COMMISSION ON FOOD ADDITIVES (VI.1.1)

Warsaw, 25-27 July 1974

Present: Dr. E. O. HAENNI (Chairman), Dr. A. E. WASSERMAN (Secretary), Prof. G. GRIMMER, Dr. F. POUILLAUDE, Dr. E. SOMERS (Titular Members); Mr. D. F. DODGEN, Dr. S. J. KUBACKI, Mr. E. A. WALKER (Associate Members).

Minutes of Previous Meeting

The minutes of the meeting in Munich on 23-25 August 1973 (see *Comptes Rendus XXVII Conference: Part B*, pp. 232-234) were approved.

Current Programme Reports

(i) Mr. WALKER presented the present status of the Collaborative Study on Nitrosamines. Eleven of the original 18 collaborators had completed the second phase of the study—analysis of nitrosamines in a canned meat sample. Several methods in current use were applicable to the analysis of volatile nitrosamines at the 20 $\mu\text{g}/\text{kg}$ level with an interlaboratory accuracy of $\pm 50\%$. Because several of the methods used might not be adequate at lower levels, it was recommended that a more critical evaluation of a meat sample at 5-10 $\mu\text{g}/\text{kg}$ nitrosamine content be carried out. At such time as it appears that a method or methods appropriate for full collaborative study were available, the Commission would recommend further active participation.

Mr. WALKER had at hand four descriptions of procedures from laboratories whose results fell within the accuracy indicated above. He proposed publication of these methods, and the collaborative results, in a manual of analytical methods for volatile nitrosamines. In discussion, concern was expressed that such publication by IUPAC might be interpreted as recom-

mentation of these methods comparable to that accorded to methods for other substances, which were based on a full collaborative study by laboratories using the same method. At the same time, it was agreed that availability of the methods might serve a useful purpose. Accordingly, the Commission recommended that the manual be published by IARC with appropriate acknowledgment of IUPAC participation. Presumably, the Section would need to obtain IUPAC approval for such publication.

(ii) Dr. KUBACKI presented his report on 'A Survey of Multi-Antioxidant Procedures in Foods', concluding that adequate qualitative procedures established by collaborative studies were available. However, he found no quantitative procedures accepted as recommended methods of analysis and proposed to complete a literature survey on such methods, preparatory to selection of a method for collaborative study.

The scope of the needed multi-antioxidant quantitative procedures should be based on actual usage of these compounds. It was proposed that the study undertaken by the National Academy of Sciences for the US Food and Drug Administration on the use of such preparations in USA should be utilized. However, to extend coverage to actual usage in other countries it was proposed to request such information from the Oils and Fats Section and the Club of European Centres for Lipid Research. On the basis of such information the Commission proposed to define the scope required for an adequate multi-antioxidant quantitative procedure. It was recommended that the proposed scope of the procedure be referred to the Oils and Fats Section for information on the Section's interest in developing, and collaborating in, a study of such a procedure. When the literature survey currently in progress was completed, the Commission would supply a copy to the Oils and Fats Section.

(iii) A preliminary report on the 'Review and Updating of Procedures for Individual Antioxidants' was presented by Dr. POUILLAUDE. With respect to new compounds, he recommended the addition of ethoxyquin and TBHQ and suggested development of the chapter on the salts of ascorbic acid, particularly ascorbyl palmitate. Dr. POUILLAUDE pointed out the significance of synergists and metal scavengers in the protection of foods against metal oxidation and suggested the addition of such products as lactic, citric, and phosphoric acids and their salts. For their description and determination the procedures were adequate as described in WHO publication Food Additive Series No. 3, 1972.

The Commission concurred in Dr. POUILLAUDE's recommendations and further recommended the publication of the new material in a supplement to the earlier IUPAC document 'Survey of Analytical Methods Available for the Estimation of Some Food Additives in Foods'. The draft should be circulated to interested member countries for comment.

(iv) Prof. GRIMMER presented his report on the procedure for Polycyclic Aromatic Hydrocarbon Profile Analysis (Multistage by GLC) of high-protein foods, oils, and fats. Having obtained the cooperation of 15 laboratories he had initiated a study using vegetable oil as a matrix for 8 PAH. Dr. HAENNI expressed concern that the sample did not contain benzo(e)-pyrene as well as benzo(a)pyrene, an omission which Prof. GRIMMER explained as being due to the exhaustion of his supply of this compound. [Benzo(e)pyrene is a potential interfering substance in the determination of benzo(a)pyrene by gas chromatography.] A new supply of benzo(e)pyrene

had been arranged. This compound would be included in the PAH to be added to a meat sample in a future study.

(v) At the joint meeting of the Fermentation and Food Sections in Munich (1973) it was agreed that Dr. HAENNI would undertake to supply information on a modified Howard procedure applicable to single cell protein. This modification had been developed by the Gulf Research and Development Corpn. It had now been learned that this laboratory had extended the procedure to multi-polycyclic aromatic hydrocarbon analysis in single cell protein and had submitted a manuscript for publication. Under the circumstances it would be inappropriate for the Food Section to disclose prematurely this procedure. It was recommended that the Fermentation Section be advised to contact Dr. M. NORRIS (Gulf Research and Development Corpn., Pittsburgh, Pennsylvania) for details of the modified procedure.

(vi) Dr. SOMERS submitted a survey for synthetic and artificial sweeteners. The survey indicated that there were available at this time adequate methods for the determination of permitted sweeteners, as well as for cyclamates and for their significant impurities. The Commission recommended publication of the survey as a useful reference source.

(vii) Mr. DODGEN presented a report on the analysis for asbestos in talcs and silicates used in foods. It was concluded that this complex problem was currently under investigation by several international agencies and there did not appear to be a significant contribution which IUPAC could make at this time. Mr. DODGEN estimated it would be at least a year before it would be appropriate to reevaluate this situation. However, he pointed out that there was an ongoing collaborative study of a microscopic method under the auspices of AOAC. The AOAC Referee was Dr. A. E. SCHULZE (US Food and Drug Administration): interested parties should communicate with him directly.

Unresolved Current Projects

(i) The project on determination of nitrite and nitrate in meat could not be pursued this year because of the resignation of Dr. RHODES, who had initiated the work. Dr. WASSERMAN undertook to proceed with the evaluation of this subject.

(ii) Prof. GRIMMER submitted a brief evaluation of the potential contamination of food by carcinogenic heterocyclic polycyclic hydrocarbons. He concluded that there was a real potential for such contamination and indicated he would initiate a preliminary study of the problem.

(iii) It was concluded after some discussion that the revised Food Chemicals Codex specification, which included a viscosity test, was adequate for control of harmful, low-molecular weight fractions for carrageenan in foods.

(iv) In the absence of Prof. H. D. BELITZ, the Commission could not effectively consider publication of the Mohler-Mayrhofer report on Nitrosatable Amines in Foods.

(v) Again, the absence of Prof. BELITZ or his representative did not permit effective consideration of the English translation of the previously presented report on specifications for thickeners and emulsifying agents in foods.

New Programmes

In addition to the work to be initiated by Prof. GRIMMER on heterocyclic hydrocarbons in food, Mr. WALKER was to prepare an evaluation of the

situation with respect to vinyl chloride migration into food from polyvinyl packaging materials, including the analytical aspects.

Diversification of Food Section Programme

The Commission disagreed with the concept that analytical aspects of the food programme should be transferred to the Analytical Chemistry Division. Aside from the question of differences in specialized analytical expertise involved, it was believed that for effective progress the analytical phases were inseparable from the other aspects of the food programme, which were commonly dependent vitally on the analytical work. This conclusion was the basic one in the Commission's view, although there was discussion of various alternative structural aspects of the Food Section work. The Commission believed these were relatively of minor importance and that a number of viable alternatives were possible.

A. E. WASSERMAN

COMMISSION ON FOOD CONTAMINANTS (VI.1.2)

Warsaw, 25-27 July 1974

Present: Dr. K. KOJIMA (Chairman), Dr. K. OHNO (Secretary), Dr. A. D. CAMPBELL, Dr. P. KROGH, Dr. P. L. SCHULLER (Titular Members); Prof. G. BILLEK, Dr. M. JEMMALI, Dr. J. D. LITTLEHAILES, Dr. P. S. STEYN (Associate Members); Dr. W. KRÖNERT (National Representative); Mr. F. BRO-RASMUSSEN (Observer).

Minutes of Previous Meeting

The minutes of the meeting held in Munich on 23-25 August 1973 (see *Comptes Rendus XXVII Conference: Part B*, pp. 235-239) were approved. In this connection Dr. CAMPBELL mentioned that the following were to be published during August 1974 as Technical Reports appendices to the *Information Bulletin*:

- No. 9 Recommended Method for Aflatoxins in Copra, Copra Meal, and Coconut
- No. 10 Development of a Method to Evaluate Sampling Plans Used to Estimate Aflatoxin Concentrations in Lots of Shelled Peanuts
- No. 11 Collaborative Study of the Determination of Aflatoxin M₁ in Milk

International Monitoring Programme for Food Contaminants

Dr. KOJIMA reported that this Programme was planned by FAO and WHO, and he had been asked to cooperate in it. In this connection, Dr. KROGH mentioned that he was invited to attend a meeting in October 1974 to discuss the technical problems of the Programme. The Commission understood that the Programme to be run by FAO and WHO might need the help of IUPAC on the best up-to-date information on analytical methods, and it agreed to furnish such information as a body to those organizations subject to the approval of the Applied Chemistry Division Committee.

Dr. KOJIMA would utilize the opportunity of his visit to FAO headquarters

to start a preliminary talk on this matter as the Chairman of the Commission.

Determination of Mercury in Food

Dr. H. GUTHENBERG reported the results of analysis of the data, including one additional result obtained after the last meeting. The Commission decided to circulate the draft of the standard method, together with the summary of results, to the Members for their comments and to consider publication.

Determination of Lead and Cadmium in Food

Dr. OHNO reported that a collaborative study was being made and five results had so far been returned out of 20 participants. Because low recoveries were observed for lead in orchard leaves and for cadmium in some samples, it was decided to call a halt to the experiments by the various laboratories, informing them of the results and comments which had come already from five laboratories, and to ask for comments on further study. Difficulties in establishing a method to be applied to various kinds of food were pointed out by Dr. SCHULLER and the Commission recognized the need of a note in the IUPAC method in this respect. Dr. CAMPBELL mentioned that the method of lead determination in milk by the US Food and Drug Administration was satisfactory and promised to submit details of the method.

Review of Available Methods for Cadmium in Food

This review has been finished by Dr. A. J. COLLINGS and could now be distributed to Members for their comments and proposals for further action.

Determination of Copper in Food

Dr. SCHULLER distributed his paper proposing revision and updating of the present IUPAC method. It was decided that comments should be sent to him by the end of November 1974, so that the revised method could be accomplished before the next Commission meeting.

Determination of Selenium in Food

A paper prepared by Dr. L. E. COLES, reviewing chemical aspects of selenium relating to public health hazard, had been distributed to the Members of the Commission, but no comments had been received. Recognizing the need for a standard method of analysis, the Commission agreed to ask Dr. COLES to prepare a recommendation of some methods so that the Commission might select one to be elaborated as a standard IUPAC method.

Determination of Fluorine in Food

The report from Prof. R. TRUHAUT had not arrived and the Commission decided to await it before considering further action.

Methods for Destruction of Organic Matter

The report prepared by the Commission on Microchemical Techniques and Trace Analysis (V.2) had been distributed for comment by the Members of the present Commission. Dr. MARCUSE reported that the Food Section had no specific comments to make. However, it was recognized that Prof. BILLEK had some comments which would be circulated to the Members of this Commission and then sent to Commission V.2.

Second IUPAC Symposium on Mycotoxins in Food

A successful Symposium was held in Puławy (23-24 July 1974), attended by 91 persons from 20 countries. Some 51 papers were submitted, of which 46 were actually read. The meeting was organized by Prof. NIKONOROW, Prof. JUSZKIEWICZ, Dr. KOJIMA, Dr. KROGH, and Dr. MARCUSE. Prof. JUSZKIEWICZ would take care of publication of the papers. If manuscripts were ready by September 1974, they would be printed next year (price *ca.* \$10).

Minicolumn Methods for Mycotoxins

Aflatoxin. The Roemer method applicable for a number of food items had been submitted for publication, and an AOAC collaborative study had just been conducted on an international basis. The results of the collaborative study would be available in August 1974 and would then be circulated to Members of the Commission. If accepted by the Commission, the Roemer method would receive IUPAC recommended status and should be published as an IUPAC Technical Report.

Ochratoxin A. A method had been developed by Hald and Krogh and submitted for publication. An IUPAC collaborative study would be conducted by Dr. KROGH. Dr. CAMPBELL would write a review on minicolumn methods, which would be circulated to Members of the Commission.

Mycotoxin Formation during Shipment of Foodstuffs

This project, already discussed at the previous meeting, had been reconsidered in view of the fact that it would be too expensive to conduct. However, the Commission felt that the project was important and that all efforts should be made to carry it out. An outline for the study would be produced, and then an effort made to find financial support. The project would be conducted by Drs. KROGH, CAMPBELL, and KRÖNERT.

International Mycotoxin Check Sample Series

A copy of the letter soliciting supplemental funds for IARC to take over the programme was printed in the May 1974 issue of JAOAC. The letter had also been sent to Members of the Food Section and would be sent to individuals who were in a position to contribute through their organizations. A special bank account had been set up for acceptance of contributions. The present committee was preparing proposed rules for the new operation, which included expanding the committee to represent the international interest.

Single Cell Proteins (SCP)

The report on SCP which had been prepared by Dr. N. R. JONES was distributed to Members at the meeting. After some discussion, tentative agreement was reached as follows. SCP were currently used only in animal feedstuffs, therefore collaborative testing for purine and nucleotide analysis would not be necessary. Concerning the amino acid analysis of SCP, it must be considered in relation to the diversification of the programme of the Food Section, *i.e.*, quality of foods. In the event of amino acid analysis being undertaken, priority might be given to some kind of human foodstuff, *e.g.*, meat or fish.

Purity Requirements for Solvents for Dispersion

The revised paper on purity requirements of seven dispersion solvents prepared by Dr. COLLINGS, would be distributed asking for comments of Members to be sent to the Chairman by the end of October 1974, the paper then to be published.

Round Table Discussion on 'Purity Requirements for Food Additives and their Standardization'

Dr. KOJIMA briefly reported on the 1973 meeting in Hamburg, and that which would be held in The Hague on 29 July 1974.

International Courses on Mycotoxin Analysis

WHO had shown a growing interest in training personnel in mycotoxin analysis. The first WHO organized course was held in Sofia during December 1973. Requests from other countries were expected. IUPAC had recommended that methods of analysis were a natural basis for the courses. WHO and FAO should be informed that IUPAC was prepared to provide expertise for these courses.

Detoxification of Mycotoxin-contaminated Foodstuffs

Detoxification was an aspect which deserved special attention. As a first step Dr. JEMMALI would prepare a status report on aflatoxin contaminated foodstuffs.

Sampling Plans for Mycotoxin Analysis

A paper on sampling plans by Whitaker and Dichens was under publication as IUPAC Technical Report No. 10 (see page 43). In addition, Dr. CAMPBELL would prepare a status report on sampling plans for aflatoxins.

Mycotoxin Residues in Food of Animal Origin

In accordance with the minutes of the last meeting, the Commission had decided to mount a collaborative study on aflatoxin and ochratoxin residues in meat. The study would be conducted by Drs. KROGH and JEMMALI.

TLC Method for Ochratoxins

During the previous meeting the Nesheim procedure for ochratoxin analysis received IUPAC recommended status. The method would be republished as an IUPAC Technical Report.

Standards for Mycotoxin Analysis

Dr. J. V. RODRICKS (US Food and Drug Administration, Washington, DC) would be asked to prepare a status report on availability and purity requirements of the standard.

Third IUPAC Symposium on Mycotoxins in Food

The matter was discussed and the general feeling was that it would be useful to organize a third Symposium in connection with the Food Section meeting in 1976.

Method for Aflatoxin M₁ in Dairy Products

The method by Stubblefield and Shannon had been studied collaboratively by AOAC. The results of the study would be evaluated by Members of the Commission by correspondence. If accepted by the Commission, the method would receive IUPAC recommended status.

Diversification of Commission Programme

(i) The proposal of the Chairman for collection of information on food contaminants derived from food packagings and containers was agreed as a project of the Commission and was decided to be proposed to the Food Section for comment. In connection with this project, Prof. BILLEK promised to prepare a working paper on available methods of analysis of vinyl chloride migrated from packaging materials.

(ii) The proposal of the Chairman on the principle of the work of the Commission on contaminants in connection with establishment of the standard method of analysis in food, to have 'chemical evaluation of contaminants' which included information on their levels in foods, sources in foods, chemical nature in foods, mechanism of concentration in foods, evaluation of accuracy of old data determined by old analytical methods, *etc.*, was accepted by the Commission, with the following comments. Duplication of work to collect information on the levels in food should be avoided. Critical examination of the data in connection with accuracy and sensitivity of the old analytical method was necessary and a general critical view on the level based on the available data should be given.

(iii) The nitrate problem in fresh vegetables was brought to the attention of the Commission and would be discussed by the Food Section.

(iv) Concerning rapid methods, Dr. CAMPBELL mentioned that one should be aware of the lapse of time using multidetection methods which could be applied to determine a number of contaminants at the same time, as well as the actual time for the analysis itself.

The Commission agreed to report the following items to the Food Section in connection with rapid methods:

(a) *Multi-analysis method for mycotoxin.* Dr. STEYN agreed to prepare a working paper.

(b) *Column combustion method for detection of mercury.* Dr. CAMPBELL enquired about the need of a rapid method for mercury in fish, and Dr. KOJIMA replied that a method using column combustion was now used in Japan and promised to send this information to the Members.

(c) *Minicolumn methods for detection of mycotoxins.* These were also rapid methods and were now accepted as official projects of the Commission.

(v) Dr. CAMPBELL called the attention of the Commission to the matter of use of animal waste for animal feed, and mentioned that this would come soon as a note on the Federal Register. It was decided to refer the matter to the Food Section.

K. OHNO

COMMISSION ON NOMENCLATURE OF INORGANIC CHEMISTRY (II.2)

Slaughan Manor, Sussex, 12-19 August 1974

Present: Prof. W. C. FERNELIUS (Chairman), Dr. D. M. P. MINGOS (Secretary), Prof. R. M. ADAMS, Prof. L. F. BERTELLO, Dr. K. C. BUSCHBECK, Prof. Y. JEANNIN, Dr. G. J. LEIGH (Titular Members); Prof. J. CHATT, Dr. W. H. POWELL, Prof. K. YAMASAKI (Associate Members); Dr. G. H. CHEESEMAN, Dr. L. C. CROSS (Observers).

1. The minutes of the meeting held in Munich during 21-26 August 1973 (see *Comptes Rendus XXVII Conference: Part B*, pp. 148-154) were approved.
2. The Chairman stated that this meeting of the Commission was particularly important, because it represented the final opportunity for making decisions which could influence the contents of the next Collective Index of *Chemical Abstracts*. Dr. POWELL indicated that suggestions for the format and content of this Index would have to be received at Chemical Abstracts Service before December 1974.
3. It was decided that the document 'Chemical Nomenclature, and Formulation of Compositions, of Synthetic and Natural Zeolites', prepared by Prof. R. M. BARRER's Zeolites Nomenclature Working Party, required no further discussion. A postal ballot had shown that the Members of the Commission were in favour of publishing this report as a Provisional Nomenclature Appendix to the *Information Bulletin*.
4. Prof. CHATT reported on the amendments made by the Commission on Nomenclature of Organic Chemistry (at its meeting in Dorking, July 1974: see page 33) to a third draft of 'Nomenclature of Isotopically Modified Compounds'. He noted that the Organic Nomenclature Commission was unlikely to approve the Boughton system as an alternative because it recommended small letters for element symbols and used IUPAC numbering procedures inconsistently.

The Inorganic Nomenclature Commission discussed the document in some detail and came to the following conclusions:

- (a) The designation of locant positions by functional group indicators was unsatisfactory and unsuitable for indicating the positions of attachment of a complex organic ligand to a metal ion.
- (b) The Commission would prepare its own document on 'Nomenclature of Isotopically Labelled Inorganic Compounds'. This document would summarize the rules given in the organic chemistry nomenclature document, but it would use inorganic compounds for illustrating the rules. Prof. FERNELIUS volunteered to prepare the first draft of the document. Drs. POWELL and LEIGH were asked to keep him informed of their deliberations on the designation of locant positions in complex ligands.
- (c) The next edition of *Nomenclature of Inorganic Chemistry* (the Red Book) would contain a more detailed discussion of isotopically modified inorganic compounds. The document which Prof. FERNELIUS was preparing would probably serve as a basis for the appropriate section.
- (d) The Commission recommended that italics be retained for element symbols because they were required for efficient computer recognition of chemical formulae.

5. The Commission reaffirmed its view that a systematic method for naming the elements with atomic numbers greater than 106 was urgently required. Theoretical speculations concerning these elements were frequently published and therefore names for these elements were required for indexing purposes. The Commission was not attempting to diminish the right of a discoverer to propose a name for a new element, but merely presenting a systematic naming system for undiscovered elements.

The Chairman was instructed to write to the President of IUPAC and to the President of the Inorganic Chemistry Division with the request that the Bureau should reconsider the proposals put forward by the Commission at Munich in 1973.

6. The Commission decided to retain the term *lanthanoid* to describe the elements from lanthanum to lutetium in the Periodic Table. It rejected the objections raised against this name by Prof. K. BAGNALL. The Chairman was instructed to communicate this decision to Prof. BAGNALL and explain that the Commission considered the term *lanthanoid* was etymologically sound and historically well founded. Prof. BAGNALL had also questioned whether the term *niccolate* would find general acceptance amongst chemists. It was agreed that the term *niccolate* had only been introduced by the Commission as a model for international usage, and that *nickelate* was an acceptable variant in the English language.

7. Prof. CHATT summarized the Organic Chemistry Nomenclature Commission's recent discussion of Section D to *Nomenclature of Organic Chemistry* ('Rules for Organometallic Chemistry') and gave a detailed account of the alterations that had been made to the tentative rules document [Tentative Nomenclature Appendix No. 31 to *Inf. Bull.* (August 1973)]. A number of decisions were reached in reply to specific requests from the Organic Nomenclature Commission.

8. Dr. POWELL gave a short talk on the way chemical formulae and names were introduced into and stored by computers. In the discussion that followed, interest was shown in the possibility of using mathematical connection tables instead of names for complex chemical compounds and the general availability of computer programmes, which could generate chemical names from connection tables.

9. The document 'Philosophy and Guidelines' prepared by Prof. FERNELIUS was discussed. Dr. LEIGH emphasized the importance of defining clearly long and short term goals. There was some disagreement about how often the Red Book needed revision. Some concern was expressed about the lack of cooperation from editors of scientific journals. The Commission was disturbed that the IUPAC journal, *Pure and Applied Chemistry*, did not insist that articles conform with IUPAC nomenclature recommendations. The Chairman was asked to write to the Scientific Editor of the Union to enquire whether a more strict editorial policy could be adopted. The Chairman commended Prof. CHATT's efforts to improve the standard of nomenclature in The Dalton Transactions of the UK Chemical Society.

The educational role of the Inorganic Nomenclature Commission was stressed by several Members. Dr. BUSCHBECK suggested that IUPAC nomenclature documents ought to state more clearly how names were derived and which system of nomenclature was being used. The Commission decided that there was little it could do, as a body, to enlarge its educational contribution. It was willing, however, to assist individual efforts by Commission

Members to introduce good nomenclature practices into school and university curricula. The Commission also decided not to publish Prof. FERNELIUS's document 'Philosophy and Guidelines'.

10. The Commission decided to publish 'Naming an Inorganic Compound' which paper had been prepared by Prof. FERNELIUS. This document would serve as a guide to the Red Book, and might be incorporated into the next edition. Comments on this document should be sent before the end of November 1974 to Prof. FERNELIUS. He would then complete and submit a final draft for publication by IUPAC.

11. Dr. CROSS reported that the Organic Nomenclature Commission had formed a working party to study the nomenclature of cations, anions, and radicals. Dr. LEIGH was nominated to join this group on behalf of the Inorganic Nomenclature Commission. Existing practices for naming inorganic cations, anions, and radicals, were summarized in documents prepared by the Chairman for the meeting.

Prof. CHATT presented his document on 'Nomenclature of Hydrides of Nitrogen and Derived Anions and Ligands'. His proposals were accepted in principle, but some minor alterations were recommended. A second draft of this document would be sent to all Members and a postal ballot organized to decide whether Members agreed to its publication by IUPAC.

12. Prof. JEANNIN presented a document which indicated some of the problems encountered when trying to name a metal cluster compound. In the discussion which followed, the Commission was unable to agree on a definition of the term 'cluster' and decided to try and prepare a document on this topic without defining it rigidly. It was generally agreed that the fluxional character of some carbonyl cluster compounds need not be indicated in their names.

Dr. POWELL presented a detailed paper from Chemical Abstracts Service on cluster nomenclature. This document seemed to overcome many of the problems noted by Prof. JEANNIN and was therefore accepted in principle by the Commission. Dr. POWELL and his colleagues were advised to change the document to include more examples of genuine metal cluster compounds. The Commission would consider a second draft at its next meeting.

The punctuation marks used in cluster names were discussed in some detail. Dr. POWELL pointed out that ligand priorities for bridging and terminal ligands were not presently defined. It was agreed that the rules must give some guidance about how to simplify the names for symmetrical cluster compounds. Also, it was noted that the -ane system of nomenclature might prove useful for naming metallo-carbane polyhedral compounds. The Secretary was asked to send the addendum of Dr. POWELL's document to Prof. A. A. VLČECK and ask his advice on the topological notation which was being suggested.

13. The documents 'Designation of Coordination Sites in Ligand Names' prepared by Dr. POWELL and 'Naming of Complexes Containing Complex Organic Ligands' prepared by Dr. LEIGH were discussed. There was general approval for the use of the Greek letter kappa (κ) for indicating the ligating atoms in ligand names. The Commission instructed Drs. LEIGH and POWELL to investigate the limitations and strengths of this system of notation. It was decided that when naming a complicated ligand in a complex compound, it was most helpful to choose a canonical structure for the ligand which was neutral. If this was not possible, the ligand canonical form with the smallest possible formal negative charge was to be preferred.

14. The Commission could not agree on a system of nomenclature for inorganic ring and chain compounds. It was agreed that a document which presented simultaneously alternative hetrane and coordination nomenclature names would be prepared by Drs. BUSCHBECK and POWELL and sent to outside experts for their opinions.

15. The Commission endorsed the views of Prof. N. LOZAC'H on the tetrapyrrole nomenclature document prepared by Prof. R. BONNETT on behalf of the IUPAC-IUB Commission on Biochemical Nomenclature. Prof. FERNELIUS had also written to Prof. BONNETT expressing the Inorganic Nomenclature Commission's position.

16. The document prepared by Prof. BERTELLO on 'Highly Fluorinated Inorganic Compounds' would be rewritten using -io radical names and then reconsidered at the next meeting.

17. The Chairman's modification of Table 2 of the Red Book was found to be generally acceptable. It was agreed that the contents of the Table should be listed alphabetically and that the reference to IUPAC and Chemical Abstracts nomenclature rules be retained.

18. Dr. POWELL and Prof. ADAMS presented substantially different proposals for boron hydride nomenclature. Dr. POWELL suggested adoption of the *debor*-system of numbering, while Prof. ADAMS favoured retention of the *nido*- and *arachno*- descriptors with these terms now defined rigidly. Dr. BUSCHBECK stated that the Gmelin Institut had published a numbering scheme for boranes and carboranes based on the *debor*- system. The Commission suggested that these three Members should work together to produce a mutually acceptable document. Comments on these documents should be sent to the Secretary by the end of October 1974.

19. The document 'Stereochemical Notation in Coordination Chemistry, Mononuclear Complexes' would be prepared for publication.

20. The following persons would be accepted as National Representatives to the Inorganic Nomenclature Commission if recommended by their respective National Adhering Organizations: Dr. T. D. COYLE (USA), Prof. E. FLUCK (Federal Republic of Germany), Prof. J. KLIKORKA (Czechoslovakia).

21. The Commission would be pleased if Dr. CHEESEMAN, a former Secretary of the Commission, could write a history of the Commission. The Chairman was asked to approach Dr. CHEESEMAN on this matter.

22. The Commission agreed that it could achieve more results if it met separately from the 28th IUPAC Conference in 1974. The Chairman was instructed to request the President of the Inorganic Chemistry Division to bring this view to the attention of the Bureau.

D. M. P. MINGOS

ANALYTICAL CHEMISTRY DIVISION EXECUTIVE COMMITTEE

Warsaw, 22-24 August 1974

Present: Prof. N. TANAKA (President), Prof. W. KEMULA (Past-President), Mr. R. W. FENNELL (Secretary).

The President asked for a period of silence in memory of Dr. A. C. MENZIES.

Division Finances

The Secretary reported that approximately \$6,500 had already been spent by the Division from its 1974 Contingency Fund and another \$1,500 was allocated for the meeting of Commission V.3 in November. It was noted that estimated expenses for the meetings of Commissions V.1, V.4, and V.5 were very close to the allocations of \$1,500. In view of possible future expenditures, the action of the Secretary in refusing at short notice, an additional allocation to Commission V.4 was approved, and it was decided not to offer financial support for meetings of any of the other Commissions.

Elections

Vice-President (President-Elect). The election of Prof. T. S. WEST (UK) as President-Elect of the Division, to take office after the 28th IUPAC Conference, was noted.

Secretary and Division Committee Members. The correspondence between the Secretary and the Chairman of the N/E Committee (Dr. M. KAPEL) was noted. It was observed that five Division Committee Members and a new Division Secretary would be taking office after the 28th IUPAC Conference. The draft procedure proposed by the Secretary to avoid nominations for more than one position on the Committee was approved.

Programme of the Division

Commission Status Reports. The Status Reports of all seven Commissions were studied in detail and the Secretary was instructed to take up specific points with the Commission Chairmen. It was agreed that the terms of reference drafted by the Commission Chairmen at the XXVII IUPAC Conference in Munich should be circulated to the Division Committee for comment, before the next Conference.

Coordination of Commission Projects. The documents relating to possible overlap of Commission projects were noted. The necessity for reference of the matter to the Division Committee was regretted. The President expected that he would receive replies by the end of October.

Commission V.2 Project—Sensitivities of Trace Analytical Methods. The progress of this project, initiated after discussion between representatives of the Analytical Chemistry and Applied Chemistry Divisions at Munich, was noted. It was agreed that the progress of this item, and particularly the involvement of other Commissions, should be reviewed by the Division Committee at the next Conference.

Publication of Reports. It had been suggested by some Members of the Division Committee that two Commission V.2 reports should be summarized in *Pure and Applied Chemistry* and published in full in specialized microchemical journals. Although known to be contrary to established IUPAC procedure, the suggestion was referred to the IUPAC Publications Committee, which had decided to try an experiment with these two reports. A synopsis of each report would be included in PAC with casual requests for photocopies of the full material to be serviced from the Secretariat. The Commission should be approached for advice as to which general and specialist journals should be invited also to include the synopsis.

It was observed that these proposals did not meet the suggestions of the

Members of the Division Committee but, as the IUPAC Publications Committee was empowered to decide how any IUPAC report should be published, it was agreed that the Commission should be asked to comply with the request for a synopsis of these reports and that the Division Committee should be kept informed of these developments.

Cooperation with the Applied Chemistry Division

Prof. TANAKA and Mr. FENNELL reported on their meetings with representatives of the Applied Chemistry Division Committee. It was agreed that the closer liaison established between the two Divisions was very encouraging and should be maintained. Prof. TANAKA would take up points of detail directly with Dr. H. EGAN, President of the Applied Chemistry Division.

Cooperation with ISO

Comments from Members of the Division Committee on the proposed scheme for vetting and possible IUPAC approval for ISO International Standards were discussed in detail. Since the XXVII IUPAC Conference at Munich there had been considerable further experience within the Division of ISO Draft International Standards, and there were some severe reservations on the ability of Members of the Division to recommend IUPAC approval on the basis of the information provided by ISO when the DISs were submitted for comment. Members of the Division Committee were reluctant to approve documents without evidence of exhaustive trials of their validity—IUPAC approval should not be given lightly—and, even if such evidence were produced, the time taken to examine ISO documents would have to be taken from that available for normal IUPAC work. Some Members of the Division Committee were, however, prepared to operate the system proposed at the Munich Conference.

In view of the current division of opinion in the Division Committee and uncertainty of the extent of involvement by IUPAC in ISO business required by the Bureau, the President agreed to seek to withdraw at the forthcoming Bureau meeting, the Division's detailed proposals for IUPAC approval of ISO Standards, in order to seek clarification of official IUPAC policy, and to raise the matter again at the next Division Committee Meeting.

Cooperation with FECS

The question of the appointment of an official IUPAC representative on the Working Party on Analytical Chemistry of the Federation of European Chemical Societies was discussed. It was agreed to ask Prof. T. S. WEST if he would act in this capacity.

Revision of IUPAC Statutes and Bylaws

Proposed revisions of the Statutes and Bylaws of the Union, reported as Appendices E and F of the Minutes of the 81st Executive Committee meeting, were discussed. The President was asked to raise certain points at the forthcoming Bureau meeting.

R. W. FENNELL

SECTION ON OILS AND FATS (VI.3)

Warsaw, 28-30 August 1974

Present: Drs. H. J. VOS (Chairman), Prof. C. PAQUOT (Secretary), Dr. H. BRÜSCHWEILER, Prof. E. L. DELVAUX, Dr. N. D. EMBREE, Dr. J. GRACIAN TOUS, Mr. A. T. MØLLER, Drs. J. C. VAN DER WEEL (Titular Members); Prof. T. ASAHARA, Dr. C. CAROLA, Dr. J. A. CORNELIUS, Prof. M. NAUDET, Mr. A. PETERSEN, Prof. A. RUTKOWSKI, Prof. H. WESSELS; Mr. J. P. WOLFF (Associate Members); Mr. S. B. LINZ CHRISTENSEN, Drs. P. W. HENDRIKSE, Prof. J. HOLLÓ, Dr. A. JAKUBOWSKI, Dr. P. R. E. LEWKOWITSCH, Mr. B. M. MCGWYNNNE, Prof. R. MONACELLI, Prof. H. NIEWIADOMSKI, Dr. R. OHLSON, Dr. J. POKORNÝ, Dr. M. TEUPEL (National Representatives); Dr. K. BABUCHOWSKI, Dr. D. CHOBANOV, Dr. A. HAUTFENNE, Dr. E. KURUCZ, Dr. K. MODZELEWSKA, Dr. H. SZCZEPANSKA, Dr. W. SZELEJEWSKI (Observers). The meeting of the Section was held in conjunction with those of the Commissions on Oils and Fats (VI.3.1) and on Soaps and Oleochemicals (VI.3.2).

Minutes of Previous Meeting

A report of the meeting held in Munich during 22-25 August 1973 had been published in *Comptes Rendus XXVII Conference: Part B*, pp. 243-245.

Membership

The Members approved the nominations as National Representatives to the Commission on Soaps and Oleochemicals by the relevant Adhering Organizations of Dr. A. HAUTFENNE (Belgium) and Dr. D. FIRESTONE (USA). It was noted that some countries active in the area of oils and fats were not yet represented in the Section or its two Commissions (Brazil, Norway, USSR, Yugoslavia). The Secretariat would be asked to contact their Adhering Organizations with a view to nominating National Representatives. The Secretary was requested to write to the President of the Applied Chemistry Division, to seek permission from the Bureau for Drs. Vos to continue as Chairman until 1977.

Chairman's Report

Messrs Butterworths had informed the Committee on Publications that loose-leaf supplements to the 5th edition (1964) of *Standard Methods for Analysis of Oils, Fats, and Soaps*, were not a viable proposition for sales purposes. Instead, it was suggested that supplementary material be published in *Pure and Applied Chemistry* as it became available, then to consolidate it into a separate publication at longer intervals. Reprints of supplementary methods in the journal might be sold from the Secretariat, it being left to purchasers whether to convert them to loose-leaf form.

The present revision of IUPAC Statutes and Bylaws envisaged that Sections attached to Divisions should be reclassified as Commissions. The Applied Chemistry Division Committee had suggested a single Commission to replace the present Section on Oils and Fats and its two Commissions. The Chairman felt that this change would concentrate the work into the hands of fewer official Members and necessitate assignment of tasks to other individuals on a less formal basis.

The Chairman and Secretary would be meeting the President of the Applied Chemistry Division later in the year to discuss these and other matters concerning the Section.

Work Programme 1973-1974

The results of the various collaborative studies were discussed. Two new methods were adopted with some modifications to be introduced in the texts of the relevant appendices to the Work Programme:

- (i) Determination of Lower Fatty Acids and/or Fatty Acid Composition of Butter Fat by Gas Liquid Chromatography (Appendix 3/74)
- (ii) Determination of Content of Isolated Trans-Unsaturated Components in Oils, Fats, Fatty Acids, and Fatty Acid Methyl Esters by IR Spectrophotometry (Appendix 6/74)

A working group (Chairman: Prof. PAQUOT) was created to prepare the final texts of these two methods, which would be published as II.D.19.4 and II.D.22, respectively.

After having adopted the principle of separate working groups for each subject, the Members agreed that the study of the other methods from the 1973-1974 Programme be continued for a further period, and that for this purpose the following working groups be established:

- (i) Determination of Melting Range (Chairman: Prof. NAUDET)
- (ii) Determination of Total Oxidized Fatty Acids (Chairman: Prof. NAUDET)
- (iii) Determination of Tocopherols in Oils and Fats (Chairman: Drs. HENDRIKSE)
- (iv) Determination of Pesticides (Chairman: Prof. DELVAUX)

Future Programme

The Chairman proposed a large programme for the coming years. Many of the studies mentioned would involve collaboration with other international organizations.

Commission on Oils on Fats

—linoleic acid content of oils, fats, and margarine:

health aspects, control aspects in connection with declaration and food laws; common interest to industry and public authorities.

—percentage of solid fat in fats by low resolution NMR (with AOCS):

control aspects; common interest to industry.

—trace metals in oils and fats (with other IUPAC bodies and AOCS):

health aspects, quality aspects in connection with stability; common interest to authorities and industry.

—polyethylene in oils and fats (with ISO):

quality aspects, health aspects in connection with migration from packaging material; common interest to commerce, industry, and authorities (food laws).

—identification and determination of emulsifiers used in food industry (with other IUPAC bodies):

control aspects in connection with food laws and Codex Alimentarius directives; common interest to authorities and industry.

—percentage of total fat in margarine:

control aspects; interest to industry and public laboratories.

—residual solvent in solvent extracted crude oils and fats (with IASC):

hazard aspects in industry, safety handling, quality and control aspects; common interest to commerce, industry, and authorities.

—*antioxidants in oils and fats by GLC* (with AOCS, ISO, and other IUPAC bodies):

health aspects, control aspects in connection with food laws; common interest to commerce, industry, authorities, and Codex Alimentarius Commission.

—*stability of oils and fats by accelerated tests* (with ISO):

comparison of the already adopted AOCS method (AOM) with the method of ISO (it was hoped that at the ISO/TC 34/SC 6/WG 3 meeting in The Hague on 23-24 September 1974, that French colleagues would give detailed information on the method proposed by them); quality aspects in connection with stability; common interest to commerce and industry.

—*pesticides in oils and fats* (if still necessary, with other IUPAC bodies, OICC and Codex Alimentarius):

health aspects, control aspects in connection with food laws; common interest to commerce, industry, and authorities.

—*minor quantities of waxy material in oils* (with IASC):

quality and control aspects; common interest to commerce and industry.

—*study of composition of unsaponifiable matter* (if possible and necessary with OICC):

quality aspects in connexion with identification of products; common interest to commerce, industry, and authorities.

—*study of changes taking place in oils and fats during deep fat frying* (as proposed by Mr. PETERSEN):

The Members were already engaged in the determination of total oxidized fatty acids. Another possibility would be the determination of dimerized and polymeric substances in heated fats and oils.

Health aspects, quality and control aspects; of great importance to food inspectors and governmental control laboratories and to industry.

—*further study of bleaching tests for oils, palm oil* (with IASC and Technical Committee of the Rubber Growers Association):

quality aspects; common interest to commerce and industry.

—*study of changes taking place during refining of oils and fats* (with special reference to deodorization at high temperatures):

health aspects, quality aspects; common interest to commerce, industry, and authorities.

—*determination of and distinction between phospholipids in oils and fats* (in collaboration with Commission VI.3.2):

quality aspects in connection with further treatment of the oils and fats; common interest to industry and commerce.

—*determination of position of double bonds in hydrogenated oils and fats*:

process control aspects; of interest to industry dealing with hydrogenation.

—*percentage of oils in seeds by low resolution NMR* (with IASC and ISO/TC 34/SC 2):

quality aspects, control aspects; common interest to commerce and industry.

—*completion of methods for oleaginous seeds and fruits* (Section I of the 5th Edition) by adopting those published by IASC, ISO/TC 34/SC 2, AOCS.

—*determination of sulfur and sulfur-containing substances*

—*drawing up of a vocabulary on oils and fats*, in the same way as had been done by the Commission of Terminology of CID.

This matter had already been discussed at previous meetings at the request of Prof. G. JACINI; realization, however, would not be easy.

—*elaboration of a dictionary on oils and fats*, giving the various characteristics, notably with regard to the natural composition.

AOCS had already done work in connection with the fatty acid composition at the request of the Codex Committee on Fats and Oils.

—*study of quality of plastic bottles in connection with the quality of oils stored in them*

Commission on Soaps and Oleochemicals

As proposed by Mr. MØLLER:

—*completion of the methods of analysis for glycerine* (Section III of the 5th Edition) *and soaps* (Section IV) by adopting those already published by other organizations like CID, AOCS, ISO/TC 91.

—*addition of standard methods for other oleochemicals*, by adopting those already published by other organizations; development and publication of those methods that were not being studied and published already elsewhere.

Before starting any study on more general problems in the field of soaps and oleochemicals, it would be necessary to dispose of methods of analysis that would guarantee useful and reproducible results.

For the period 1974-1975, the following working groups were established:

- (i) Determination of Content of cis-cis Linoleic Acid in Oils and Fats by an Enzymatic Method (Chairman: Dr. Ö. LEVIN)
- (ii) Determination of Oil Content of Seeds by Low Resolution NMR (Chairman: Mr. WOLFF)
- (iii) Analysis of Frying Oils (Chairman: Prof. WESSELS)
- (iv) Identification and Determination of Emulsifiers (of Fatty Origin) in Oils, Fats, Fat Products (Margarine, Sauces, Mayonnaises), Cosmetics (Chairman: Mr. MØLLER).

Publications

It was agreed to publish some 20 methods recently adopted by the Section as a Fourth Supplement to the 5th Edition of Standard Methods, preferably in loose-leaf form rather than in *Pure and Applied Chemistry*. A working group was created (Chairman: Prof. PAQUOT) to prepare a new 6th Edition. Total revision of the methods included in the 5th Edition and the First Supplement (1966) was envisaged.

Date and Place of Next Meeting

The Section and its Commissions would meet next during the 28th IUPAC Conference (Madrid, September 1975).

C. PAQUOT

COMMISSION ON SPECTROCHEMICAL AND OTHER OPTICAL PROCEDURES FOR ANALYSIS (V.4)

Washington, DC, 2-4 September 1974

Present: Prof. V. A. FASSEL (Chairman), Mr. B. F. SCRIBNER (Secretary), Prof. C. TH. J. ALKEMADE, Mr. L. S. BIRKS, Prof. J. D. WINEFORDNER (Titular Members); Mr. R. JENKINS (Associate Member). The meeting was an interim one, with limited attendance from Commission Members, in order to progress selected nomenclature documents.

1. The document 'Nomenclature, Symbols, Units and their Usage in Spectrochemical Analysis-II. Terms and Symbols Related to Analytical Functions and Their Figures of Merit' [Tentative Nomenclature Appendix No. 26 (November 1972) to *Inf. Bull.*] had been reviewed at the Commission meeting in Munich in 1973 (see *Comptes Rendus XXVII Conference: Part B*, page 193). A new draft, prepared by Mr. BIRKS and Mr. SCRIBNER, was circulated to the Commission in June 1974. At the present meeting, the draft was revised and it was now believed to be in acceptable final form. This draft would be retyped in Prof. FASSEL's office within 10 days, then circulated within the Commission. A question remaining to be resolved by the full Commission was the advisability of including the Appendix listing equations involved in making corrections for inter-element effects.

2. The document entitled 'Nomenclature, Symbols, Units and their Usage in Spectrochemical Analysis-III. Analytical Flame Spectroscopy and Associated Procedures' [Tentative Nomenclature Appendix No. 27 (November 1972) to *Inf. Bull.*] had been prepared in revised form (dated June 1974) in the Chairman's office and circulated. This draft and comments received were thoroughly reviewed. The resulting corrections, mostly editorial, were to be incorporated by Prof. ALKEMADE and the document then forwarded to Prof. FASSEL for typing and distribution to the Commission.

3. Part IV of the series of nomenclature documents 'X-Ray Emission Spectroscopy' had been prepared in revised draft (dated December 1973) by Mr. BIRKS and circulated to the Commission at that time. At the present meeting the draft and comments received were reviewed. Recommendations were made for changes, especially for conformance to recognized IUPAC symbols for general terms. Mr. BIRKS would prepare a new draft incorporating the recommendations and circulate it within the Commission as soon as practicable.

4. It was noted that efforts to publicize Part I of the nomenclature series ['General Atomic Emission Spectroscopy', *Pure Appl. Chem.* **30**, 651-680 (1972)] were having some success. It had just been republished in *Applied Spectroscopy* **28**, 398-410 (July/August 1974).

5. The Chairman called attention to the importance of considering the future Membership of the Commission, because several vacancies would occur at the close of the present period (1973-75). Suggestions of names for consideration of appointment to the Commission should be forwarded to the Chairman.

6. The Commission intended to meet at the 28th IUPAC Conference (Madrid, 1975), with sessions on 3-6 September. At that meeting the entire programme of the Commission would be reviewed and documents approved

where appropriate. Special effort should be made to circulate any drafts within the Commission with allowance of time for review before the meeting.

B. F. SCRIBNER

SECTION ON MEDICINAL CHEMISTRY

Noordwijkerhout, 8-9 September 1974

Present: Prof. E. J. ARIËNS (Chairman), Dr. A. I. RACHLIN (Secretary), Prof. A. ALBERT, Dr. L. G. HUMBER, Dr. M. PROTIVA, Prof. P. SENSI, Dr. J. THUILLIER (Titular Members); Dr. J. F. CAVALLA, Dr. F. MARTIN, Prof. E. MUTSCHLER, Prof. S. SAREL (Associate Members); Prof. M. CARMACK, Prof. W. TH. NAUTA (Observers).

The Chairman called for a moment of silence in memory of Prof. E. E. SMISSMAN.

Minutes of Previous Meeting

The minutes of the meeting held in Munich on 23-25 August 1973 (see *Comptes Rendus XXVII Conference: Part B*, pp. 165-169) were approved.

Committee on Education

The final report of the *ad hoc* Committee on Education of Medicinal Chemists, prepared under the Chairmanship of the late Prof. SMISSMAN and largely moulded by him, had been issued as Technical Report No. 13 (August 1974), an appendix to the *Information Bulletin*. The IUPAC Secretariat had been requested to send copies to all Section Members, correspondents, and sundry interested parties. This list would now be expanded to include FIP and IUPHAR. The availability of this document would also be announced in the next Section Newsletter. It was decided to retain a reconstituted Education Committee which would issue a second report in approximately 3-4 years. The posture of this sequel would be determined largely by feedback which would be solicited from recipients of Technical Bulletin No. 13. For the near term the education of medicinal chemists would be a continuing Section project which would be incorporated, in some form, into future Section-sponsored scientific meetings. A goal would be a practical short course of instruction to be offered in London at the time of the VI International Symposium on Medicinal Chemistry, which was being planned for 1978. An effort would be made to have some preliminary plans ready for discussion at the time of the V International Symposium on Medicinal Chemistry, scheduled for Paris in 1976.

Prof. ARIËNS appointed the following group as members of the reconstituted Education Committee: Prof. NAUTA (Chairman), Dr. CAVALLA (Secretary), Prof. COMBET-FARNOUX, and Prof. MUTSCHLER. Prof. ALBERT, Prof. BURGER, and Prof. PRATESI were named as advisers to the Committee.

Committee on Symposia and Meetings—Long Range Planning Committee

The discussion involving these two *ad hoc* Committees soon converged, which led to the obvious decision to reconstitute them as a single body to be known as the Long Range Planning Committee. This Committee would keep the Section aware of new developments in medicinal chemistry: it would en-

deavour to anticipate those areas requiring study and action by the Section; it would attempt to anticipate future subjects for timely symposia and conferences and to stimulate groups to sponsor international medicinal chemical symposia on these topics. Also to be promoted would be meetings in areas not necessarily of immediate interest, but of concern to the world at large and the underdeveloped countries in particular. A typical example would be tropical diseases involving experts in all facets of a given disease, including clinical personnel, marketing and distribution experts, *etc.* Possible subjects for consideration would be solicited in the Newsletter.

Prof. ARIËNS appointed the following group as members of the newly defined Long Range Planning Committee: Dr. CAVALLA (Chairman), Prof. MUTSCHLER (Secretary), Prof. CAMPAIGNE, Prof. SAREL, and Prof. SENSI. Prof. ALBERT, Prof. BURGER, and Prof. ARIËNS were appointed advisers to the Committee.

Committee Concerned with Predictions of Quantitative Structure-Activity Relationships on Patent Problems

Dr. HUMBER, Chairman of this *ad hoc* Committee, gave a brief overview of the background to the problem, a synopsis of the Committee's report, and its recommendations. The following discussion centred mainly on how the report should be disseminated and particularly to whom it should be directed. Concerning distribution, the IUPAC Secretariat would be approached about the possibility of publishing the entire report as a Technical Report or alternatively, as an insertion in a future IUPAC *Information Bulletin*. It was also decided that the report should be distributed to working medicinal chemists and patent agents. Dr. HUMBER and his Committee were thanked and congratulated for their splendid effort. Minor revisions would be made in the latest draft and the final copy would be sent to the Secretary by 15 October. The availability of the report would be announced in the Newsletter and comments would be solicited.

Reports on Symposia and Meetings

XI International Symposium on Chemistry of Natural Products (Ottawa, 1974). This IUPAC meeting was cosponsored by the National Research Council of Canada and the Chemical Institute of Canada (CIC). Of 18 industrial sponsors, 16 were major pharmaceutical companies. The Medicinal Chemistry Division of CIC was involved in the planning from the outset and the programme had three sessions of particular interest to medicinal chemists. Dr. HUMBER reported that the meeting was heavily attended and an unqualified success, which supported the contention that significant medicinal chemistry content could be included in future IUPAC Natural Products Symposia.

25th IUPAC Congress (Jerusalem, 1975). Prof. SAREL reported that the second bulletin had been issued. In addition to regular accommodations, plans were being made to provide about 500 student residences in order to attract younger people to the Congress. The medicinal chemistry programme would comprise six major symposia and four microsymposia at different locations. Topic selection had been made very carefully in order to supplement rather than duplicate recent symposia.

V International Symposium on Medicinal Chemistry (Paris, 1976). Plans were in the preliminary stages and Dr. THUILLIER was concerned mainly with obtaining guidance from the Section on such matters as timing, duration,

format, topics, etc. It was recommended that the meeting be held for 4 days in the latter half of July 1976. Considerable discussion regarding format indicated preference for the usual mix of plenary lectures by recognized authorities and short presentations. Regarding the latter, consideration would be given to the 'poster' approach to allow more participation and full discussion. A notice soliciting topics would appear in the next Newsletter. The Secretary would also contact the IUPAC Secretariat immediately regarding IUPAC sponsorship.

VI International Symposium on Medicinal Chemistry (London, 1978). In his preliminary report, Dr. CAVALLA said that this meeting would be organized by a subcommittee of the UK Society for Drug Research. Current plans were directed at a university location with attendance limited to 750 people. The UK Chemical Society, UK Pharmaceutical Society, and FIP would be kept informed and their collaboration would be sought. A positive move in this direction had already been made with IUPHAR. In view of the recommendation made at the present meeting to provide a short course on teaching medicinal chemistry in conjunction with this Symposium, Royal Institute of Chemistry collaboration in organizing the course would be sought.

Communications

Relationship with WHO. Because there were many instances when the interests of the Medicinal Chemistry Section coincided with some activity of WHO, the question arose as to the possibility of having a liaison member on a permanent basis rather than *ad hoc*. This question would be brought to the attention of the IUPAC Secretariat for clarification.

Newsletter. The Newsletter continued to be an important function of the Section. Currently, about 190 primary mailings were made, but hundreds of copies were duplicated and distributed by various adhering groups. Dr. RACHLIN repeated his request for suggestions as to change of format and for more contributions from individual members.

European Journal of Medicinal Chemistry. This journal, the successor to *Chimie Therapeutique*, was now accepting papers for publication in English, French, and German and, as a consequence, it was becoming an increasingly more important organ for scientific communication among medicinal chemists. A suitable announcement of this development would be inserted in the Newsletter.

Cooperative Projects with Other Groups

Infrared-Raman Spectral Data and Solubility Data. At the last Section meeting Prof. ALBERT was commissioned to gather information regarding the compilation of data on pure compounds of medicinal interest, specifically the approximately 500 compounds listed in the International Pharmacopoeia. Contact was made with the Coblentz Society and the IUPAC Infrared and Raman Spectroscopy Sub-Commission (I.5.1) and also the IUPAC Solubility Data Sub-Commission (V.6.1). Whereas all parties expressed interest, none of them, including the Medicinal Chemistry Section, had the financial backing to provide the compounds for measurement. On further discussion it developed that tables of these data would actually be of little practical value and the expenditure of the tremendous amount of time, money, and effort, required to compile these data could not be justified. These projects would not, therefore, be pursued.

Data Flagging Project. The IUPAC *ad hoc* Interdivisional Working Party on developing a Data Flagging System under the direction of Prof. D. N. HUME was judged to be a viable and useful effort. Prof. ALBERT's contact with Prof. HUME was formalized and he would act as the Section liaison with the Working Party. He was charged with ensuring the inclusion of flags of importance to medicinal chemists. The Secretary would distribute the existing list to all Members and correspondents, who would be requested to send any suggestions pertaining to this project directly to Prof. ALBERT.

Collaboration with Outside Groups

Cooperation with IUPHAR. The Section had been approached by IUPHAR representatives early in 1974 to have a Member participate in certain IUPHAR meetings as an observer and to collaborate in various other ways. Prof. ARIËNS had appointed Dr. CAVALLA to serve in this capacity at meetings held in the London area and himself or an alternate at other locations. This arrangement was approved with enthusiasm.

Cooperation with FIP. Cooperation with FIP similar to that with IUPHAR had long been in effect on an informal basis through the good offices of the Netherlands correspondent, Prof. NAUTA. This cooperation was approved and Prof. NAUTA was encouraged to continue and strengthen the relations with FIP through its President, Dr. J. WINTERS.

Contact with Prof. A. BURGER. Prof. ARIËNS had been approached by Prof. BURGER, retired editor of *Journal of Medicinal Chemistry*, with an offer to assist the Section in any capacity. Because of his vast experience, Prof. BURGER could be very helpful in many ways and consequently his offer was accepted. He had already been appointed as an adviser to the Education and Long Range Planning Committees. In his correspondence Prof. BURGER indicated several areas where the Section could be active and indeed, unknown to him, the Section had already taken action on all but one. The remaining point, his suggestion that a publication on reviews be sponsored, was not accepted. Instead, it was proposed that Prof. BURGER, because of his long editorial experience, could do a great service to medicinal chemistry by contacting the editors of the various journals dealing with this subject with the objective of bringing them together, perhaps at the time of an international symposium, for an exchange of ideas and views. Ultimately, a counterpart of the Association of Editors of European Chemical Journals, headed by Dr. L. C. CROSS (UK), might be established. Prof. BURGER would be requested to consider this suggestion and, if he reacted positively, to contact Dr. CROSS for advice and to report back to the Section.

Next Section Meeting

The Membership deplored the notice received from the IUPAC Executive Committee that the Section would not be permitted to move its 1975 Meeting from the 28th IUPAC Conference site (Madrid) to the 25th IUPAC Congress site (Jerusalem). It was emphatically pointed out that many of the Members, being extremely active in their respective scientific disciplines, would participate in the Jerusalem Medicinal Chemistry Programme which would be of the highest calibre. The unfortunate timing of the Madrid Conference so much later than the Congress would preclude attendance by several Section Members at Madrid because of the loss of too much time and also, in the case of Associate Members, for financial reasons. Because it appeared certain

that the Section would have a large delegation in Jerusalem, it was decided to conduct an unofficial business meeting at the time of the Congress and to withhold finalization of the decisions and minutes until final discussions with those Members who would attend the official meeting in Madrid.

Reply to IUPAC Concerning Areas of Activity and Financial Support

At the XXVII IUPAC Conference, Prof. CAMPAIGNE in his capacity of Section Chairman, made certain suggestions to the IUPAC authorities regarding areas of potential activity and possible sources of financial support from trusts and foundations. A letter had subsequently been received expressing certain viewpoints and requesting some documentation from the Section. After discussion it was decided that this matter could best be handled by letter from Prof. ARIËNS to the Executive Secretary.

New Business

Food Additives. There was a discussion precipitated by the ever increasing concern over toxicity arising from longterm exposure to food additives, either deliberate (*i.e.*, anti-oxidants, *etc.*) or incidental (*i.e.*, plasticizers from packaging materials, *etc.*). It was concluded that this matter, being constantly monitored by the WHO-FAO Committee on Food Additives, was not a primary concern of the Section. However, there were certainly many instances where the chemical expertise and experience of its Membership could be of great value. Prof. ALBERT was commissioned to contact the WHO-FAO Committee with an offer of such cooperation and assistance when requested.

Problems of Drug Control. The question of drug control, being a timely topic particularly among lay people, was discussed with the aim of finding a way in which a group such as the Section could make a positive contribution. It was concluded that this matter was beyond its capability and must be handled by governmental agencies.

Section Election. In line with the election procedure applied in Munich in 1973, an election would be held to fill those Titular Member vacancies which would arise in 1975 and to elect an entirely new set of Associate Members as of 1975. As in the past, this would be organized and conducted by the Secretary.

Seeking Divisional Status in IUPAC. In reply to a question raised as to the status of the Section in IUPAC, the Secretary recounted the history of this body from its inception. It was understood that the status of a Section of IUPAC was similar to that of a Commission, and the latter were intended to be temporary bodies. The opinion was expressed that the present group had been extremely active from the onset, had certainly demonstrated its viability, and consequently might qualify as a Division. It was decided to approach the Bureau for elevation to Division status and the Secretary was instructed to make the necessary enquiries.

A. I. RACHLIN

MACROMOLECULAR DIVISION COMMITTEE

Madrid, 16 September 1974

Present: Prof. H. BENOÎT (President), Prof. C. G. OVERBERGER (Vice-President), Prof. G. SMETS (Secretary), Dr. R. F. BOYER, Prof. E. W. FISCHER,

Prof. V. A. KABANOV, Dr. A. J. DE VRIES (Members); Dr. J. W. BARRETT, Dr. H. CHERDRON, Dr. H. EISENBERG, Prof. A. J. STAVERMAN (Coopted Members); Prof. W. J. BAILEY, Prof. C. H. BAMFORD, Prof. J. KÁLAL, Prof. J. KOPS, Prof. J. J. LINDBERG, Prof. I. M. PANAYOTOV, Prof. B. RÅNBY, Prof. P. SIGWALT, Prof. A. SILBERBERG, Prof. F. TÜDÖS, Prof. E. TURSKA (National Representatives); Prof. G. W. BECKER (Representative of IUPAP); Prof. P. CORRADINI, Prof. J. FONTÁN, Prof. E. B. MANO, Prof. D. C. PEPPER (Observers).

Minutes of Previous Meeting

The minutes of the meeting held in Munich on 22-23 August 1973 (see *Comptes Rendus XXVII Conference: Part B*, pp. 170-173) were adopted without change.

Macromolecular Symposia and Microsymposia Sponsored by IUPAC

1974. The President expressed the thanks of the Division Committee to Prof. MANO for the splendid organization and high scientific level of the Macromolecular Symposium held in Rio de Janeiro during July 1974. Also, he expressed his gratitude to Prof. FONTÁN, Chairman of the 23rd International Macromolecular Symposium currently taking place in Madrid, for the organization of that meeting, and presented his best wishes for a completely successful Symposium. The President reminded the Members of the Division Committee of three microsymposia sponsored by IUPAC in 1974, namely on

Cross-Linking and Networks (Prague, 26-29 August)

Discussion Conference on Heterogeneities in Polymers (Mariánské Lázně, 2-5 September)

II Aharon Katzir-Katchalsky Conference: Biopolymer Interactions—Workshop on Physical Chemistry of Biologically Active Assemblies (Amsterdam, 2-6 September)

From the opinions of Members of the Division who had attended these particular meetings, they were all very successful, and the organizers should be congratulated.

1975. The Chairman of the 24th International Symposium on Macromolecules (Jerusalem, 13-18 July 1975), Prof. SILBERBERG, gave additional comments and information about its organization and the main topics of the scientific programme.

Three microsymposia would also be held in 1975. The Macromolecular Division agreed to recommend IUPAC sponsorship for each of them:

Polymerization of Heterocycles (Ring-opening) (Jablonna, 23-25 June; Chairmen: S. PENCZEK and P. REMPP)

Modified Polymers, their Preparation and Properties (Bratislava, 24-27 June; Chairman: A. ROMANOV)

Degradation and Stabilization of Polyolefines (Prague, 21-25 July; Chairman/Secretary: J. POSPISIL)

1976. Two official requests for IUPAC sponsorship of microsymposia had already been received:

II Microsymposium on Photochemical Processes in High Polymers (Leuven, June 1976; Chairman: G. SMETS)

II Microsymposium on Polyvinylchloride (Lyon-Villeurbanne, 5-9 July; Chairman: A. GUYOT)

The Macromolecular Division agreed to recommend that sponsorship be granted to both meetings.

Prof. RÅNBY intended to organize a symposium on Weathering, Ageing, and Degradation of High Polymers in Stockholm, just before/after the symposium of the Rheological Society. The Macromolecular Division Committee was favourably inclined to this initiative; its final agreement would be given as soon as an official information questionnaire was introduced at the IUPAC Secretariat.

Also, Prof. KÁLAL hoped to organize one or two microsymposia in Prague in 1976. The titles of these meetings would be confirmed in the near future.

1977. Final agreement had already been given for the organization of the 26th IUPAC Congress in Tokyo. On that occasion, an international macromolecular symposium was foreseen with active participation of the Division.

1978. The International Macromolecular Symposium would be in USSR, very likely in Tashkent. A final decision from the Soviet authorities was expected within a few months. The proposal for this meeting was made by Prof. KABANOV.

1979. The International Macromolecular Symposium would be organized in Federal Republic of Germany. A proposal to this effect was introduced by Prof. FISCHER, Dr. CHERDRON, and Prof. BECKER.

The proposal of Prof. PEPPER (Ireland), concerning organization of a Macromolecular Symposium in Dublin, was also considered favourably. The possibility of organizing such a meeting in 1977 was suggested, considering that participation in the Tokyo Congress would necessarily be limited on account of the high travel expenses involved. It was suggested, however, that the topics chosen for the Dublin Symposium should differ from those of the Tokyo Symposium.

The President also informed the Division Committee about a proposal from Dr. MICHAËLI and Dr. A. EISENBERG (Israel) concerning the organization of a microsymposium devoted to Ions in Polymer Systems. Considering that this subject was included within the topics of the 1975 Jerusalem Symposium, it was agreed to postpone the introduction of a formal application until the informal Division Committee meeting in Israel (July 1975).

Election of New Members (Madrid, 1975)

Division Committee. Considering the Statutes and Bylaws of the Union and the present list of official Members of the Macromolecular Division Committee, only Prof. BENOÎT and Prof. OVERBERGER would remain after the 28th IUPAC Conference (as Past-President and President of the Division, respectively). All other Members had to be replaced unless one of them was elected as Vice-President or Secretary of the Division.

It was agreed that the Secretary should send a letter to all Members of the Division, asking for nomination of candidates to be introduced at the IUPAC Secretariat before 31 May 1975, with a *curriculum vitae* of the candidate not exceeding one page. A list of those nominated would then be distributed to all voting Members before the end of June 1975.

In agreement with the Bylaws (4.105), the Division Committee should choose from among its Members, a Vice-President designated as President-Elect, not later than 2 years before assuming the Office of President, and a

Secretary. These elections were subject to approval by the Council.

Commission on Macromolecular Nomenclature. In accordance with the Bylaws of the Union all Titular Members, except for Prof. N. A. PLATÉ and Dr. W. RING, would complete their periods in 1975. However, in order to ensure continuity of the work, the Division Committee would suggest to the Bureau that Dr. K. L. LOENING, Dr. R. B. FOX, Prof. P. CORRADINI, and Prof. T. TSURUTA should stay on for 2 more years. Consequently, three vacancies would have to be filled, for which the names of Prof. N. M. BIKALES (USA), Prof. A. D. JENKINS (UK), and Prof. P. SIGWALT (France) had already been suggested.

Commission on Polymer Characterization and Properties. The composition of this new Commission was examined and the names of four Titular Members suggested, namely Dr. BARRETT (Chairman), Dr. BALL, Dr. DE VRIES, Dr. WILSKI.

Activities of Working Parties

A report on the activity of the Working Party on Structure and Properties of Commercial Polymers was presented by its Chairman, Dr. DE VRIES, and approved unanimously by the Division Committee. An afternoon session of the Madrid Symposium would be devoted to discussion of two reports from this Working Party.

J. MEISSNER: 'Basis Parameters, Melt Rheology, Processing and End-use Properties of Three Samples of Low Density Polyethylene'

J. L. S. WALES: 'A Collaborative Study of Capillary Flow of a Highly Lubricated Unplasticized Polyvinylchloride'

and a report from the Working Party on Molecular Characterization of Commercial Polymers

C. STRAZIELLE: 'Characterization of High Density and Low Density Polyethylene'

Education in Polymer Science

Concerning the investigation on Education in Polymer Science (former report of Prof. SMETS), it was desirable that all Members of the Division should provide Prof. SMETS with the addresses of existing national polymer groups and available documentation concerning this subject.

G. SMETS

COMMISSION ON ELECTROCHEMISTRY (I.3)

Brighton, 20-21 September 1974

Present: Prof. R. HAASE (Chairman), Dr. R. PARSONS (Vice-Chairman), Prof. G. MILAZZO (Secretary), Prof. I. EPELBOIN, Prof. N. IBL, Prof. A. SANFELD, Prof. E. YEAGER (Titular Members); Dr. J. C. JUSTICE (Associate Member).

1. The minutes of the previous meeting (Munich, 22-24 August 1973) had been published in *Comptes Rendus XXVII Conference: Part B* (pp. 127-128).

2. Prof. MILAZZO gave an introduction emphasizing the possibilities of electrochemical investigation in nonisothermal systems for the purpose of scientific knowledge and its practical application. After a thorough discussion in which all Members participated, it was decided that:

- (i) the Commission should include electrochemistry in nonisothermal systems among the projects of its future activity;
- (ii) an enquiry should be carried out to find the names and addresses of scientists interested in this field. All Members should communicate to Prof. MILAZZO the name and address of any scientist known to work in this field.
- (iii) the Secretary General of the International Society for Electrochemistry should be contacted to explore the possibility of holding a special session devoted to 'Nonisothermal Electrochemistry and its Applications' during (or immediately before or after) the 1976 ISE Meeting.

3. Prof. EPELBOIN discussed the difficulty of distinguishing primary from secondary inhibitors. Because of the interest shown by several scientists he suggested that a symposium be held on this theme, but that the Commission should not consider this project, for the time being, among its activities.

4. DR. PARSONS reviewed the present position of Appendix III to the *Manual of Symbols and Terminology for Physicochemical Quantities and Units*, devoted to 'Electrochemical Nomenclature' [*Pure Appl. Chem.* **37**, 499-516 (1974)]. He considered Appendix III only as the conclusion of the first stage of this project. The subsequent discussion was concluded with the decision that such nomenclature reports should constitute one of the major activities of the Commission and should be continued in the form of smaller detailed reports, each one devoted to a field of particular interest for electrochemistry. It was also suggested that small intercommission groups be formed, of not more than two persons from each interested Commission. These groups should work out the nomenclature and terminology in areas of common interest which would then be submitted to the relevant parent Commissions. The Chairman was charged to contact the Chairmen of Commissions I.1, I.6, and V.5, to explore the practicability of such joint work.

5. The project on collection of data on electrode kinetics by Dr. R. TAMAMUSHI was reviewed. The tables had been revised several times, but were now ready for publication, with an introduction modified by Dr. PARSONS. This project was finally approved and it was decided to send a letter of appreciation to Dr. TAMAMUSHI.

6. Continuing a wider discussion on the collection of data in general and on the basis of a communication by Dr. TAMAMUSHI that a group of Japanese electrochemists was being constituted to continue the work on collection of electrode kinetics data, opinions were expressed on the relative merits of collections containing the largest possible number of data which had been critically examined and those containing a much smaller number of critically selected data. It was stated that both types of collection were useful and that they were complementary one to another. It was then suggested to constitute, if possible, smaller groups of scientists having the task to prepare homogeneous criteria for critical selection of data, starting from general collections like those by Dr. TAMAMUSHI and Prof. MILAZZO (see Item 7). An enquiry should be carried out to explore the feasibility of this suggestion.

7. The discussion continued with the Tables on Standard Electrode Potentials presented by Prof. MILAZZO. These Tables were started as a project of the Commission immediately after the XXIV IUPAC Conference (Prague, 1967) and were discussed during their progress at subsequent Meetings of the Commission [Cortina d'Ampezzo (1969), Paris (1970), Washington,

DC (1971), Munich (1973)]. The author was always considering constructive criticism, remarks, and suggestions, by colleagues of the Commission, as well by highly qualified electrochemists outside the Commission (Prof. I. M. KOLTHOFF, Prof. N. TANAKA, *etc.*). The Tables were now in final form ready for publication. On the basis of the decision of the Commission taken at the XXVII IUPAC Conference, these Tables would be published outside the Union, preceded by an appropriate statement of the work done within the Commission. Concerning the Plambeck collection of data, the Commission recognized that this was a completely private work by Prof. J. A. PLAMBECK, without any intervention by the Commission (see minutes of Munich meeting, 1973). Resuming the suggestion mentioned under Item 4, Prof. YEAGER recommended as an activity of the Commission compilations of critically selected data on electrode potentials and related thermodynamic data. He would submit to the Commission practical proposals within the next 2 months.

8. Together with Dr. P. RUETSCHI (representative of ISO), discussions were carried out to try to coordinate electrochemical definitions and terminology of common interest for IUPAC and ISO. It was agreed to exchange documents and to remain in contact.

9. The priorities in activity of the Commission were then discussed. Following a proposal by Profs. EPELBOIN and MILAZZO, two kinds of activity were identified: shortterm (one year) and longterm projects. Among the short-term projects it was suggested and accepted that the following reports (in the sense of Item 4) be prepared and circulated in time for discussion at the 28th IUPAC Conference (Madrid, 1975):

- Interfacial phenomena in electrochemistry (Prof. SANFELD)
- Transport phenomena in electrochemical systems (Prof. IBL)
- Rate constants and transfer coefficients (Dr. PARSONS)
- Conductance, with first collection of data (Dr. JUSTICE)

Other projects (nonisothermal electrochemistry, continuation of general collections of data, compilation of smaller collections of critically selected data) were considered longterm projects and for the time being left to the individual initiative of the Members concerned.

10. The problem of the new Membership elections then came up for discussion. It was suggested to send proposals for nominations to the Secretary before 31 December 1974. He would circulate these proposals before any contact was made with the candidates nominated.

11. The advantages of the constitution of an Interdivisional Commission covering physical electrochemistry, analytical electrochemistry, and applied electrochemistry including electrochemical engineering, were then discussed. It was decided to postpone further action until more information was available.

12. The last point concerned the time schedule for the Madrid Conference in 1975. It was decided to ask the IUPAC Secretariat to allow for two whole-day and one half-day sessions of the Commission and for joint meetings with Commission I.6 and with Commission V.5.

G. MILAZZO

COMMISSION ON QUANTITIES AND UNITS IN CLINICAL CHEMISTRY (CQUCC)

Giessen, 25-27 September 1974

Present: Dr. R. DYBKAER (Chairman), Prof. R. HERRMANN, Prof. P. MÉTAIS, Mr. J. C. RIGG (Titular Members).

1. The sessions were to be considered as a joint meeting of CQUCC and the Expert Panel on Quantities and Units (EP on QU) of the IFCC Committee on Standards.

2. The minutes of the previous meeting [Munich, 18-20 April 1974: see *Information Bulletin* No. 48 (October 1974), pp. 33-35] were reviewed and approved.

3.(i) Dr. B. H. ARMBRECHT had circulated an NBS Bulletin on SI Units. Introduced the use of analytical figures of merit (IUPAC Inf. Bull. App. No. 26) into the US Food and Drug Administration and the question was now in active discussion. A series of short articles was in preparation for publication in JAOAC. Comment was being prepared for Proposed Rule Making on Diagnostic Products. The manuscript he had sent for submission to JAOAC had been divided into several separate notes.

(ii) Dr. DYBKAER had spent much time on a many-sided correspondence on quantities and units in enzymology (see Item 4). Furthermore, among others, the following had been subjects of letter exchange:

IUPAC glossary on quantities and units (support)

Argentine Congress on Clinical Biochemistry (June 1975) Symposium on Quantities and Units (documents)

IUPAC Sub-Commission on Solubility Data (support)

IUPAC data flagging (preference for descriptors)

DIN 58963, Kuvetten für photometrische Messungen (comments)

Commission QU of SFBC, Rec. aux Auteurs (comments)

Zender: Definitions in Quantities and Units (comments)

IUPS glossary for thermal physiology (comments)

(iii) Prof. HERRMANN reported that the Austrian-Swiss-West German paper on Quantities and Units had been published in *Z. klin. Chem.* The Draft discussed under Item 8 had been made up from different sources (ARMBRECHT, HERRMANN, MÉTAIS, RIGG) and comments. Some difficulties of nomenclature had arisen in Normenausschuss of BRD between spectroscopists plus clinical chemists and illumination scientists.

(iv) Prof. MÉTAIS said that the draft (Item 8) had been thoroughly studied in a nomenclature group of the French Association of Clinical Biologists. The French AFNOR studied spectrometry nomenclature and had produced a text 'Spectrometrie d'Absorption Moléculaire: Apareillage' that would be useful for Part 4 of the CQUCC spectrometry document. As regards introduction of SI in France, (i) *Ann. Biol.* had produced an Instruction to Authors requesting use of SI, (ii) government agencies would receive a note on SI, (iii) a large paper was being produced for biologists (*cf.* Australian pamphlet SI and You). Furthermore, documents on reference methods and analytical figures of merit were in preparation. Prof. MÉTAIS suggested that CQUCC English documents should contain French and German translations of the kind of quantity names. This was accepted unanimously.

(v) Mr. RIGG reported that his translation of HERRMANN's draft material for

Parts 1 and 4 (Item 8) had taken most of his time. Furthermore, he had prepared a large UNESCO publication: bibliography on the preparation and presentation of documents containing scientific and technical information, one large section of which listed recommendations on symbols for quantities and units, and presentation of numeric data.

4. The problem of quantities and units in enzymology had been much debated as a result of (i) Dr. M. ROTH's letter to the IFCC Executive Board suggesting that the relevant part of the IUPAC-IFCC Recommendations 1973, presently submitted for approval by the IFCC Council, was wrong, (ii) the CEBJ Circular 154 of a draft proposing the CQUCC-EP on QU approach instead of the previous CBN position in Rec. 1972; this circular was an outcome of the 1974 CBN meeting (see page 24). The position of ROTH was vigorously supported by the IFCC Committee on Standards' Expert Panel on Enzymes and by Prof. G. GORIN as theoretical spokesman. At the moment all decisions were pending on the IFCC Executive Board meeting at Harrow (October 1974), the CBN-CEBJ meeting in UK (1975), and the IFCC meeting in Toronto (July 1975). The Commission was unanimous in affirming that the presentation given by the Chairman in a letter to Prof. HØJGAARD JENSEN (1974. 5. 30) was the viewpoint of the Commission. An amended version was produced for presentation at the IFCC meeting in Harrow.

5. The proposal of the ISO/TC 12 Advisory Panel of the symbol I (Roman numeral one) for unity was discussed. The Members were unable to suggest a better solution even if some problems might occur with mistaking for letter I. The Chairman would write to ISO/TC 12 accordingly.

6. The following additional references to quantities and units were noted:—

J. FREI and K. LAUBER: Recommendations internationales pour une standardisation logique de l'expression des résultats en chimie clinique. *Schweiz. Z. med. techn. Laborfachpersonal* **1**, 227-233 (1974).

J. FREI, K. LAUBER and W. BÜRGI: Recommendations de la Société suisse de chimie clinique pour une expression logique des résultats en chimie clinique. *Bull. Soc. suisse Chim. clin.* **13**, 13-30 (1972).

P. MÉTAIS: Communiqué de la Fédération Internationale de Chimie Clinique sur la nomenclature internationale en chimie clinique 1972. *Ann. Biol. clin.* **32**, 99-100 (1974).

O. SIGGAARD-ANDERSEN: Review and comments on 'International Standard. ISO 31 Series. Technical Committee ISO/TC 12, Quantities, Units, Symbols, Conversion Factors, and Conversion Tables'. *Clin. Chem.* **20**, 727-728 (1974).

7. The drafts by Dr. ARMBRECHT and by Prof. HERRMANN of 'Quantities and Units in Clinical Chemistry: Kinds of Quantities for Optical Spectroscopy—I. General Principles' were discussed in detail, unified, and extensively revised. A new draft would be written by Mr. RIGG for circulation and comment by Members.

8. The draft on 'Transport of Components with Time' was discussed during an evening meeting of Mr. RIGG and Dr. DYBKAER who would take another look at the document before renewed presentation at the next CQUCC meeting.

9. The available material on Kinds of Quantities in Absorption Spectrometry was reviewed and a sequence of presentation was decided.

10. No progress had occurred in the field of pH, activity, *etc.*, due to pre-occupation with Item 7. It was decided that a physical chemist would be needed for proper evaluation of these problems.

11. Three possible places for the next Commission meeting were discussed: Giessen, Utrecht, Wageningen. The provisional dates would be 18-21 March 1975. IFCC would be asked for the necessary funds, possibly including the attendance of an extra *ad hoc* Member who would later become a full Member.

12. The Commission would meet in Madrid at the 28th IUPAC Conference, probably during 3-6 September 1975, and possibly include a short joint meeting with Commission I.1.

13. The following documents would be produced under the cover title 'Quantities and Units in Clinical Chemistry. Optical Spectrometry':

(i) General principles (Draft 4 in preparation by RIGG)

(ii) Molecular spectrometry of liquid and solid systems

[MÉTAIS was responsible for Draft 2, which should include: 1. Absorptiometry with cuvettes. 2. Fluorometry with cuvettes. 3. Nephelometry, including turbidimetry. 4. Reflectometry. Kinds of quantities of the following types should be included: Internal transmittance (τ_i), internal absorptance (a_i), internal (decadic) absorbance (D_i , A), logarithm of internal (decadic) absorbance ($\lg D_i$), internal absorption coefficient (K_i), logarithm of internal absorption coefficient ($\lg K_i$) and analogously for 'specific' (α) and 'molar' (ϵ) concepts]

(iii) Molecular and atomic emission and absorption spectrometry in physico-chemical plasma (Draft 2 by HERMANN)

(iv) Specifications of spectrometers (RIGG responsible for making translation into English of an AFNOR document and DIN material, and for collecting earlier comments from the Commission. MÉTAIS and HERRMANN should work on the structure and logical order of the document)

Dr. DYBKAER would revise the document mentioned in Item 8.

14. As decided earlier, Dr. ARMBRECHT and Prof. MÉTAIS should continue in CQUCC after September 1975 as Associate Members. A new Titular Member would be proposed. Dr. DYBKAER would sound out two candidates in sequence as to their willingness as soon as possible and preferably already as observers at the meeting in March 1975. With an affirmative answer in hand the Chairman would contact the Section President. Dr. DYBKAER would transfer Chairmanship to the new Titular Member as soon as possible and the Commission would ask that DYBKAER be continued as Titular Member until 1977. Mr. RIGG would become Secretary as soon as possible, probably in July 1975. Hitherto the Chairman had doubled as Secretary. The next Titular Member to add would, probably, have to be one trained in physical chemistry.

R. DYBKAER

SECTION ON AIR QUALITY

Paris, 25-27 September 1974

Present: Mr. J. L. MONKMAN (Chairman), Prof. R. G. SMITH (Secretary), Dr. M. FUGAŠ, Prof. W. PILZ, Prof. R. TRUHAUT (Titular Members); Prof. C. BOUDÈNE, Prof. P. W. WEST (Associate Members), Prof. R. BOURDON

(Secretary) and Dr. S. S. BROWN attended as representatives of the new Commission on Toxicology of the Clinical Chemistry Section, for the purpose of encouraging cooperation and avoidance of overlap between the two Sections.

1. A report of the previous meeting (Munich, 22-26 August 1973) had been published in *Comptes Rendus XXVII Conference: Part B*, pp. 247-249.

2. Dr. BROWN acquainted the Air Quality Section with plans for the proposed lead symposium to be organized in 1976 by the Toxicology Commission. The basic outline was distributed and a discussion held of the proposed topics. It was the Section's understanding that the emphasis of this symposium was to be on lead in biological matrices, with particular emphasis on blood lead analysis as it might be practised by clinical biochemical laboratories, hospital laboratories, *etc.* It was intended to stress the great importance of quality control in assuring the reliability of such analyses. Also to be discussed were analyses related to lead exposure, such as certain enzyme systems, haeme precursors, *etc.* During the discussion Prof. PILZ presented the table below, based on projections made by Dr. HAENSCHLER, and showing clearly a trend towards greater reliance on biological determinations for evaluating exposure to toxic substances.

Distribution of Analyses made to Evaluate Occupational Exposure to Toxic Substances

	Actual		Projected
	1963	1973	1983
Air	92%	70%	11%
Blood	2%	12%	9%
Urine	6%	18%	80%

This led to a discussion of the interrelationship between the Air Quality Section and the Commission on Toxicology, summarized as follows. Until recently the Section on Air Quality had, in fact, been primarily concerned with occupational exposure to toxic substances, and had stressed both air and biological analyses. However, when the Toxicology Commission was formed in 1973, all former toxicological activities of the Section on Air Quality were to be terminated by that body and transferred as necessary to the new Commission. Members of the Air Quality Section did not believe it was possible nor desirable to comply literally with this change, and both Dr. BROWN and the Air Quality Section Members agreed on a restatement of the division of duties, which recognized certain necessary limitations in the activities of the Commission on Toxicology and which were discussed by Dr. BROWN. In essence, Dr. BROWN stated that the Toxicology Commission was concerned only with subjects such as environmental and occupational lead exposure which were truly largescale problems, and which required analyses that lend themselves to automation, and which further were likely to be practised by clinical laboratories throughout the world. The Commission was specifically not interested at this time in the large number of substances (such as less common metals, solvent vapours, toxic gases, and countless organic compounds) which were the daily problems confronting

many professional industrial hygienists and toxicologists. Dr. BROWN agreed, for example, that the Toxicology Commission would not be able to concern itself with the details of methods for vanadium, thallium, TDI, *etc.*, for which air and biological sample methods were presently under consideration by the Air Quality Section. The Commission would be interested in the determination of an enzyme such as cholinesterase, however, which would likely be performed by clinical laboratories.

As a result of these discussions, the Air Quality Section unanimously recommended that it should continue to concern itself with biological specimen analyses, along with air analyses and air quality, both in relation to the work place environment and the general atmosphere. Close liaison should be maintained between the two groups and minutes of meetings exchanged.

3. Among the many substances with which the Section was currently concerned, airborne sulfate particles were considered to be of the greatest importance at this time. Several sampling and analytical methods proposed and/or published by Prof. WEST and Mr. MONKMAN were currently under consideration, but it was the opinion of the Section that the subject of airborne sulfate particles or acidic aerosols was sufficiently important that it should be considered a worldwide problem justifying special action by IUPAC. Prof. WEST and Mr. MONKMAN advanced the principal arguments, which in summary concerned the ever increasing emission into the general atmosphere of such particles due to the combustion of sulfur-containing fossil fuels and the newly-created problem of sulfate emissions resulting from the widespread use in USA of catalytic converters on 1975 model-year automobiles. Presumably, it could be predicted that in time the use of such converters might be required by other countries in addition to USA. Whereas in the past gasoline combustion had resulted in the emission of relatively small amounts of sulfur dioxide, the converters now caused the transformation of this gas into sulfuric acid and/or sulfate aerosol, which was generally considered to constitute a much more serious health and environment pollution burden. Prof. WEST felt strongly, in fact, that after a sufficient number of automobiles had been equipped with catalytic converters, perhaps within 2-3 years, a very serious atmospheric situation would arise in urban areas of high traffic density.

The problem was further complicated by the fact that analytical methods traditionally used for sulfate or sulfuric acid determinations might be substantially in error, and reliable methods which did yield the required information were only now being published, but not yet in widespread use. Several such methods were being considered by the Section and would be recommended for publication, but the total problem concerned with production and effects of the aerosols on air quality, as well as methods for sampling and analysis, was sufficiently important in the opinion of the Section that a special international symposium on the subject was justified. It therefore recommended that discussion took place regarding such a symposium, and both Prof. WEST and Mr. MONKMAN agreed to investigate sources of support such as NATO, NSF, or other agencies which made it possible to underwrite the symposium. Although such a symposium could be held in any of a number of suitable locations, Mr. MONKMAN offered to be host to such a meeting in Ottawa and the suggested date was early in 1976.

4. Prof. WEST distributed a revised version for the preamble of *Analytical Methods for Use in Occupational Hygiene*, the compendium published by the Section. Some discussion concerning his draft ensued, and Prof. WEST

agreed to make certain minor revisions, then resubmit the draft to the Chairman. Some discussion was held on the delays experienced through Messrs. Butterworths in publishing eight methods approved by the Section some time ago, but which had not as yet appeared in print. Various means to speed publication were discussed, including the possibility of publishing in outside journals.

5. The remainder of the meeting was devoted to discussions of sampling and analytical methods for the following toxic substances in air and biological matrices:

Nitrogen Dioxide in Air	Sulfuric Acid Mist in Air
Carboxyhaemoglobin in Blood	Sulfates in Air
Haemoglobin Methaemoglobin in Blood	Vinyl Chloride in Air
Trichloroacetic Acid in Urine	Lead in Air
Phenol in Urine	Hydrazine in Air
Phenol in Air	Desmodur 44 in Air
Ring Oven Analyses	Desmodur 15 (1,5 -Naphthylene Diisocyanate) in Air
Carcinogens in Air	Thiophenol in Air
(i) 4-aminobiphenyl	Epsilon Caprolactam in Air
(ii) Benzidine	Pyridine in Air
(iii) β -Naphthylamine	Vanadium
(iv) Dimethyl Hydrazine	Hydrogen Peroxide in Biol Samples
(v) α -Naphthylamine	Mineral Oil in Air
(vi) MOCA	Nicotine in Air

Specific assignments and technical discussions would be sent to all Members in a separate document, after a meeting to review these matters between the Chairman and the Secretary.

R. G. SMITH

SUB-COMMISSION ON CALIBRATION AND TEST MATERIALS (I.4.1)

Warsaw, 1-2 October 1974

Present: Dr. D. AMBROSE (Acting Chairman), Dr. E. BRUNNER, Dr. J. H. S. GREEN, Dr. A. JUHÁSZ, Prof. G. MILAZZO, Prof. T. PLEBANSKI (Members); Prof. A. BYLICKI, Dr. A. MACZYNSKI, Dr. T. YOLKEN, Dr. W. ZINKE (Observers).

1. A report of the meeting held in Munich on 22-25 August 1973 had been published in *Comptes Rendus XXVII Conference: Part B* (see page 132).

2. A report by the Sub-Commission's editor, Dr. E. F. G. HERINGTON, had already been circulated. The report was to the effect that six sections of *Recommended Reference Materials for Realization of Physicochemical Properties* had been received by Dr. HERINGTON, viz.

General Introduction	(CALI)
Enthalpy	(COX)
Optical Refraction	(BROWN and LANE)
Optical Rotation	(BROWN and LANE)
Reflectance	(FEUERBERG)
Surface Tension	(BROWN and LANE)

The first five of these had been edited and passed for printing; they were expected to appear in *Pure and Applied Chemistry* 40(3), (1974). Messrs. Butterworths had been asked to send proofs to the individual authors, who were requested to forward their corrections through Dr. HERINGTON. Dr. AMBROSE reported that some difficulties had subsequently arisen with the section on Reflectance and this had been withdrawn from printing.

3. The expectation at the Munich meeting had been that the Recommendations would be issued in preliminary form as Appendices to the *Information Bulletin* for comment, but in fact the sections that had been completed were to be published immediately in *Pure and Applied Chemistry*. Other Commissions of IUPAC would not, therefore, have any opportunity to comment before publication. It was thought that no difficulties would arise with the Recommendations already in press, but it was agreed that in future each section must be sent to any other Commissions which might have an interest in the subject.

4. To avoid any possibility of confusion in future, it was agreed that sections for publication must be sent to the Chairman. He would be responsible for ensuring that each section had been approved and would then pass it to Dr. HERINGTON for editing.

5. Dr. BRUNNER offered to have copies made of papers if authors found difficulty in doing it themselves. For distribution in preparation for the meeting in Madrid (2-11 September 1975), the closing date for receipt of a paper by BRUNNER was set at 1 July 1975.

6. Dr. AMBROSE drew attention to the fact that although there was no fixed limit to the size of the Sub-Commission, it had evolved so that its Members were the section team leaders. Each team leader had the responsibility of deciding whom he ought to consult in the work he was doing and whom he needed to enrol as members of his team.

7. With regard to the naming of commercial firms as suppliers of reference materials, Dr. AMBROSE reported that after the meeting in Zeist [see *Inf. Bull.* No. 44 (December 1972), pages 37-40], he had sought the advice of the President of the Physical Chemistry Division on the subject. The Sub-Commission agreed that the disclaimer regarding sources of supply in the General Introduction should be repeated when appropriate in sections published subsequently.

8. It was agreed

- (i) that the introduction to each section should include relevant definitions and mathematical relations of the property under consideration,
- (ii) that although the Recommendations should preferably be expressed in SI units, the factors to convert these units to others commonly used should be given in each section.

It was recognized that the sections already passed for publication might not all conform with these decisions.

9. The decision was made in Zeist in 1972 that the original format used in the preparation of the Recommendations, viz. a separate sheet for each reference material, should be retained for publication. Nevertheless, it now appeared that adherence to this would sometimes lead to excessive repetition of identical statements. It was agreed therefore, that for some properties where this might occur (e.g., when a series of materials differed only in

respect of their certified viscosities), a more condensed presentation should be adopted.

10. The first batch of Recommendations would be published with the Introductory chapter in which readers were invited to comment and make suggestions for additional reference materials. It was agreed that a similar invitation should be repeated when further sections of the Recommendations were published subsequently.

11. It was noted that at a conference held in Washington in November 1973 sponsored by the Organisation Internationale de Métrologie Légale it had been agreed, in conformity with the nomenclature adopted by this Sub-Commission, that the term 'Standard Reference Materials' should become 'Reference Materials'.

12. In connection with the General Introduction, Prof. MILAZZO contended that the classification into Primary Substances (PS) and Calibration and Test Materials (CTM) ought to be expanded, and a third class introduced. In view of the lengthy discussion of this point at earlier meetings, as a result of which the number of classes was reduced from three to two, and the fact that the chapter was now in press, it was felt that there was no point in reopening the matter.

13. The relationship of the work of the Sub-Commission to the *Catalog of Physicochemical Standard Substances* [*Pure Appl. Chem.* **29**, 597 (1972)] was discussed, and it was apparent that different authors had different views about the matter. If a property of a material depended on certification (e.g., viscosity), the Recommendations were seen as extending the Catalog. On the other hand, for properties where all the recommended materials were substances which could in principle be specified in terms of purity (e.g., PVT), the question for the author was not the availability of certified samples but selection of the values to be attributed to the property. From this point of view the availability of certified samples was not a necessity, it was merely a convenience to the user, and the Recommendations and the Catalog were seen as entirely independent. There was then no reason why the former should include all the materials listed in the latter.

Because the title of the Catalog must be altered on account of the word 'Standard', it was agreed to suggest to Dr. J. P. CALI that, in line with the name of the parent Commission (I.4), it should be called 'Catalog of Reference Materials for Physicochemical Measurements from National Laboratories'.

14. Individual sections were discussed as follows (the names of the team members are given with the team leader first).

Density (BROWN)

A final draft submitted by Dr. I. BROWN was approved for publication, subject to small changes to be made by the Editor.

Viscosity (PLEBANSKI, BRUNNER)

Prof. PLEBANSKI presented a first draft on which he had already received comments from Dr. MARVIN (NBS), and he proposed to redraft it in consultation with MARVIN for consideration in Madrid. It was agreed that the title should be 'Viscosity of Liquids' and that gases should be treated separately, but that liquids at high temperatures should be included if possible (Dr. BRUNNER would assist). In the next draft a more condensed form would be adopted for presentation of the data.

It was agreed that, for inclusion in the Recommendations, reference materials must be chemically identified, *i.e.*, that a liquid of certified viscosity was not acceptable if the supplier did not state its chemical type. A supplier provided reference materials for viscosity which were certified on the basis of cooperative work in several laboratories, and were, therefore, in a different category from other commercial samples. Dr. JUHÁSZ reported that his Institute undertook calibration work in respect of viscosity, an aspect of reference materials that had not previously been noted by the Sub-Commission.

PVT Properties (AMBROSE, ANGUS)

Dr. AMBROSE presented a draft that he considered to be essentially complete, although it had inconsistencies arising from the fact that different parts had been written at different times. Dr. YOLKEN handed over additional information about some high temperature reference materials available from NBS. Dr. AMBROSE intended to write a new draft in time for the Madrid meeting.

Thermal Conductivity (ZIEBLAND, BRUNNER)

Dr. ZIEBLAND had sent a report on the enquiries he had made from Members of the Sub-Commission and the parent Commission about the reference materials available in different countries. The meeting found some difficulty in deciding what the Recommendations should cover, because the low thermal conductivity of insulating solids concerned building technology rather than physical chemistry. Nevertheless, measurements needed to be made, and special reference materials of low thermal conductivity were being produced, *e.g.*, at NBS. Dr. ZIEBLAND would be asked to continue work in liaison with Dr. BRUNNER, and to revise for Madrid the draft already written by the latter.

Vapour-Liquid Equilibria (BRUNNER, BYLICKI)

Dr. BRUNNER presented a draft revised in accordance with discussions in Munich. It was felt, however, that the introduction needed to be expanded and that the function of the analytical methods now included should be clarified. The title should be 'Vapour-Liquid Equilibria (Distillation Column Performance)'. Dr. BRUNNER agreed to redraft the material by the end of the year so that it could be circulated for comment. Prof. BYLICKI expressed his wish to help.

Hygrometry (PLEBANSKI)

Prof. PLEBANSKI presented a first draft, on which Dr. WEXLER (NBS) had already commented, and he proposed to redraft it in consultation with WEXLER for consideration in Madrid. A point made by WEXLER was that although certified reference materials were available, they were not essential for the realization of this property, and this was accepted. Prof. PLEBANSKI requested submission of any further comments by 31 December 1974, and he would invite WEXLER to become coauthor if he so wished.

Reflectance (MILAZZO, JUHASZ, YOLKER)

This paper had been temporarily withdrawn from publication because it had been learned that reference materials for this property were available in both USA and Hungary, and it was therefore incomplete. It was agreed that reconsideration of its content was required before it was published.

Optical Properties: Absorbance and Wavelength (MILAZZO)

Prof. MILAZZO presented drafts which were approved, but it was agreed that before publication they must be sent for comment by the Commissions on Molecular Structure and Spectroscopy (I.5) and on Spectrochemical and other Optical Procedures for Analysis (V.4).

Dielectric Constant (KIENTITZ)

In the absence through illness of Prof. H. KIENTITZ, there was nothing to report.

Potentiometric Ion Activity (CALI, DURST)

This section, written by Drs. R. A. DURST and J. P. CALI had been sent to Dr. HERINGTON with a view to its publication. The latter had reported that the section gave rise to great difficulties in presentation because various national pH scales were in use, *e.g.*, American, British, German, Hungarian, Japanese, but all were slightly different. Therefore, it was difficult to present a unified document. The meeting took the view that because measurements were being made reference materials should be recommended, and referred the section back to Dr. CALI with the request that he reconcile the differences as well as was possible. The finished version would then be referred to the Commissions on Electrochemistry (I.3) and on Electroanalytical Chemistry (V.5) for their views. It was noted that the existing draft gave special emphasis to NBS and that reference materials from other sources were not listed adequately. Comments and omissions should be sent to CALI by 31 December 1974.

Temperature Test Materials (KIENTITZ)

Dr. BRUNNER tabled a first draft by Prof. KIENTITZ and agreed to send copies to Members, who were asked to submit their comments to KIENTITZ by 1 March 1975.

Molecular Weight (GREEN)

Dr. GREEN, who was appointed team leader in February 1974, stated that he had received all the previous work and had plans to continue it. He would aim to complete this by March 1975. He intended to distribute a draft for comment before the Madrid meeting, and would establish liaison with the Macromolecular Division.

Pressure (BRUNNER)

Dr. BRUNNER had not yet started this topic and sought advice on the range of pressures and the techniques to be covered. No clear conclusions were reached and it was left to him to use his own judgement in preparing a first draft, for which the target date would be 1 March 1975. Comments should be sent to him by 1 May 1975.

Electrical Conductivity (JUHÁSZ)

After discussion of the scope of the subject, *i.e.*, whether it should include anything other than solutions of electrolytes, Dr. JUHÁSZ undertook to cover it as widely as he could by 1 March 1975. He would establish liaison with the International Electrical Commission.

15. In discussion of any omissions, it was noted that the subjects of absorption and extraction had not yet been considered, but it was decided that any more comprehensive consideration must be left for the next meeting.

D. AMBROSE

MACROMOLECULAR DIVISION WORKING PARTY ON STRUCTURE AND PROPERTIES OF COMMERCIAL POLYMERS

Ludwigshafen, 28-29 November 1974

Present: Dr. A. J. DE VRIES (Chairman), Dr. M. E. CARREGA (Secretary),

Dr. G. AJROLDI, Dr. G. G. A. BÖHM, Mr. C. BONNEBAT, Dr. H. W. BREE, Dr. C. B. BUCKNALL, Dr. J. CHAUFFOUREAUX, Dr. P. CLEGG, Mr. S. D. EAGLETON, Dr. M. FLEISSNER, Mr. A. GHIJSELS, Dr. J. HEIJBOER, Dr. R. JACOB, Dr. P. J. LAURIJSEN, Dr. H. MÜNSTEDT, Dr. J. MEISSNER, Dr. H. H. MEYER, Dr. A. PLOCHOCKI, Dr. W. RETTING, Dr. S. TURNER, Dr. A. K. VAN DER VEGT, Dr. J. ZELLINGER. A number of observers were present from BASF Research.

Meeting held at Brussels (21-22 February 1974)*

Mr. EAGLETON handed over to the Chairman the final report on the Orientation in Polystyrene programme prepared by Dr. T. T. JONES. The Chairman would submit this report for publication in *Pure and Applied Chemistry* (PAC). The final report on LDPE Rheology by Dr. MEISSNER had been accepted for publication: Prof. H. BENOÎT had suggested this report be published in the same issue of PAC in 1975 in which the plenary lectures from the 1974 Madrid International Symposium on Macromolecules were issued.

The final report on the PVC Rheology programme presented in Madrid by Mr. J. L. S. WALES was ready for publication after a slight modification concerning the comparison of the results on dynamic viscosity obtained by Rhône-Progil and Hoechst. The report would be sent shortly to all participating members in the programme and submitted for publication in PAC.

Structure and Properties of Oriented Rubber-modified Polystyrene

All participating members had received the final programme written by Dr. RETTING (27 August, 1974). Interim reports containing the first results were distributed at the meeting by AJROLDI, HEIJBOER, DE VRIES, and ZELLINGER. Further results were reported by BUCKNALL, FLEISSNER, and RETTING.

The following points were discussed extensively:

General characterization of the raw materials. The results presented on the molecular weight distribution, T_g , gel content, swelling index, solution viscosity, melt rheology, and morphology, indicated that the two samples differed sufficiently in morphology, gel content, and T_g , in order to be used in the proposed programme, although the polystyrene matrix in both materials was significantly different in MWD from the two polystyrene samples (A and B) supplied by Monsanto for the first programme. It was decided that:

HIPS VPK would be called sample I

and HIPS 475 K (commercial polymer) sample II

The two samples contained the same rubber vs pure polybutadiene with 10% vinyl content.

Flow properties determined by Rhône-Progil and Montedison were in good agreement: the difference between the samples could be explained for the greatest part by the difference in T_g .

Structure and Morphology. Observations on the structure and morphology of the elastomeric phase were presented by several laboratories. Size distributions in the two samples were slightly different; sample I contained a large number of particles of irregular shape.

Particle shape after elongation had been studied by Rhône-Progil and

*See *Information Bulletin* No. 48 (October 1974), pp. 26-29.

Cranfield; measured axial ratio was lower than the one calculated from the draw ratio.

Orientation and orientability. The methods of uni- and biaxial orientation as well as the determination of frozen-in entropic stresses used by Rhône-Progil were presented by Mr. BONNEBAT. Copies of the talk given in Paris (June 1974) by Dr. DE VRIES, describing these methods in some detail, were distributed to the members. The frozen-in entropic stress which was uniquely related to birefringence (also in the case of biaxially stretched HIPS) varied as a function of recoverable strain in accordance with the statistical theory of rubber elasticity. Calculated values of shear modulus G decreased with increasing stretching temperature, due to the breakdown of network structure. At identical values of $T - T_g$, shear modulus G was slightly higher for sample II.

Some shrinkage force measurements on oriented specimens supplied by BASF, were presented by Dr. ZELINGER. As expected, shrinkage force increased with nominal draw ratio.

Mechanical properties. Results on tensile properties and on dynamic mechanical properties were presented by Dr. ZELINGER, TNO, and Hoechst. The difference in mechanical properties between the nonoriented samples I and II might be explained partly by the presence of oil, but mainly by the higher gel content in sample II. Concerning the significance of the latter parameter, Dr. AJROLDI drew attention to a paper by CIGNA and BIGLIONE [*Proc. 2nd Meeting Ital. Soc. Rheol.* (1973), page 523]. The discussion showed that some difference of opinion existed between the members as to the relative importance of the two factors. The difference in location and height of the rubber damping peaks, measured by TNO, was certainly significant and required further explanation; this might also be true for the small secondary peak at a temperature slightly higher than T_g (rubber), visible in sample II at 1 Hz.

The peculiar variation of the transverse Young's modulus as a function of Nominal Draw Ratio, seemed to indicate that the orientation of the specimens did not correspond to a pure uniaxial extension; the latter conclusion was confirmed by the free shrinkage measurements of TNO, which clearly showed that at the higher values of NDR, some transverse orientation in the specimens was also present, in particular for sample II. As pointed out by Dr. DE VRIES, the amount of biaxial stretching might be calculated from the free shrinkage results in two directions, given in the report from TNO (the data for PS II, 6 showed, for example, that the decrease in width during stretching had been more than 20% lower than it would have been for a purely uniaxially stretched specimen). This small amount of biaxial stretching was not surprising in view of the high width-to-length ratio of the specimens before stretching (VAN DER VEGT) and might also explain, perhaps, some of the anomalies in the tensile properties, measured by Drs. ZELINGER and FLEISSNER. Drs. BUCKNALL and AJROLDI drew attention to the effect of molecular orientation on the mechanism of yielding in tensile tests (local necking or crazing); it was important, therefore, not only to supply numerical data of yield stress and strain, but also to give information on the shape of the stress/strain curve during testing and to make sure that the observed value of total elongation was not affected by local necking of the specimen.

In order to enable Drs. RETTING and ZELINGER to prepare their progress report before the 1975 Autumn Meeting of the Working Party, all participating Members were requested to send their interim reports (in English) with final results before 1st July 1975.

At the Autumn meeting the progress report would be discussed and, if necessary, amended before final publication. It was recalled that only SI-units were to be used; the units indicated on page 8 of the letter by Dr. RETTING (27 August 1974) are not the official ones as described in ISO recommendation R 1000.

Mechanical Properties of PVC

Dr. CHAUFFOUREAUX presented the actual status of the programme: the first part concerned with a detailed study of the tough-tough transition in tensile tests at low strain rates, was practically finished. Both Solvay and BASF had performed temperature measurements in the part of the specimens where yielding and ultimate rupture took place. A considerable local increase of temperature had been measured, as a function of strain rate, specimen thickness, and time. Dr. RETTING was completing his report on the work done by BASF and would finish it before the end of 1974. Dr. CHAUFFOUREAUX would prepare the final report on this part of the programme which should be ready to be submitted for publication before Summer 1975.

The second part of programme was concerned with the effect of calibrated defects (fillers) on the mechanical properties of rigid PVC. Reports and results were presented by Solvay, TNO, Montedison, ICI, and Dr. ZELINGER. ICI had made a detailed study of the quality of the extruded sheets and the tensile specimens. It was concluded that for specimens cut with their principal axis in the extrusion direction, thickness variations were negligible and should not affect the accuracy of the tensile test results. Dynamic mechanical properties had been measured by TNO, Solvay, Montedison, and Prague: fillers affected mainly the value of the modulus; the effect on damping, if any, was small. Tensile properties measured by ICI, TNO, Prague, and Solvay, were markedly influenced by filler content and/or filler particle size, in particular elongation at break and tensile impact strength. Creep measurements by ICI showed that at larger values of strain, fillers decreased the time-dependent modulus which, according to TURNER, might be explained by the lack of adhesion between filler particles and polymer matrix. In general, the effect of fillers on tensile properties seemed to decrease with increasing temperature. Dr. CHAUFFOUREAUX presented results obtained by electron microscopy which indicated that the small particle-size fillers were partly agglomerated. The results of Solvay on impact strength of prestressed specimens seemed to indicate that crack propagation was slowed down by the presence of fillers, independently of particle size.

The importance of static and dynamic fatigue tests, longterm creep and intermittent loading in creep tests, for a better understanding of the effect of fillers, was discussed extensively. Further results obtained by this type of test, in particular from ICI, were expected to be available within a year and would be discussed at the 1975 Autumn meeting. Interim reports were to be distributed at least one month before the meeting.

Rheology of Block Copolymers

Samples of Cariflex TR 1102 had been distributed by Dr. VAN DER VEGT to all participants in the programme. A first interim report from BASF had been received and was discussed at the meeting: melt flow index, technical tensile tests, and cone-and-plate measurements showed an important effect of residence time at 190°C.

According to Dr. VAN DER VEGT and Mr. GHIJSELS, the residence time effect was most probably due to crosslinking of the polybutadiene as a result of oxidation. All measurements at temperatures above 170°C should be performed in the complete absence of oxygen. Protection against oxidative attack was more critical for rotational viscosimetry (large contact area) than for capillary measurements. In the latter case it was recommended to alternate high and low shear rate measurements in order to remove the plug of cross-linked material liable to be formed at the exit of the capillary. Addition of extra amounts of antioxidant with the aid of a solvent was not recommended, because of the difficulty to remove completely the solvent afterwards. The material was also sensitive to UV and should always be stored in the dark.

In order to be sure that no crosslinking had occurred during the measurements at higher temperatures, it was recommended to check the reversibility with temperature. It should be remembered that domain size and structure were also influenced by temperature and thermal history and it was important therefore to keep a record of all experimental details.

Dr. VAN DER VEGT would send to all participating members a copy of the paper by MIERAS and WILSON with indication of the sample comparable to Cariflex TR 1102. He asked all participating members to include in their interim reports not only the graphs and figures but also the numerical data.

A first progress report containing a survey of all available results would be prepared by Dr. VAN DER VEGT and Mr. GHIJSELS before the 1975 Summer meeting of the Working Party. Interim reports from participating members were to be sent to Dr. VAN DER VEGT before 1st May, 1975 in order to be included in the survey. Members who were not able to send their interim reports before that date, should distribute them in any case at least 2 weeks before the meeting (*i.e.*, 1st June).

Some preliminary results obtained in capillary and cone-and-plate flow presented by Mr. GHIJSELS showed the expected behaviour of viscosity as a function of shear rate: a large negative slope (~ -1) at low shear rates ($<0.1 \text{ s}^{-1}$) followed by a much smaller slope, which gradually increased again in the region of high shear rates. Dr. LAURIJSEN reported preliminary results obtained in capillary flow at 150°C as a function of L/D ratio and in tensile tests at constant velocity or under constant load as a function of temperature.

As to the tensile tests during which neither stress nor strain rates were kept constant, it was observed that results should not be presented in terms of 'tensile viscosity', the latter being a clearly defined rheological parameter.

Dr. BÖHM indicated that Firestone would perform measurements in orthogonal rheometer flow (flow between eccentric rotating disks) as well as studies of morphology changes as a result of shearing.

Membership

Dr. H. E. SCHROEDER (Elastomer Chemicals Department of Du Pont de Nemours, Wilmington) had expressed his laboratory's interest in becoming a member of the Working Party. The Chairman read out the letter he had written to Dr. SCHROEDER, in which the activities and objectives of the Working Party as well as the requirements for becoming an active member were stated as clearly as possible. It was agreed that a similar letter should be sent to all future applicants for membership.

Dr. HEIJBOER drew attention to the paper on rheology of the IUPAC-PVC compound presented by COLLINS and NAKAJIMA at the recent annual meeting of the Society of Rheology. All members agreed that the procedure

followed by GOODRICH was not in accordance with the practice of the Working Party and that the Chairman should remind COLLINS of the existence of the Rule which stated that members no longer able to participate actively, were invited to resign from membership. It was noted indeed, that B. F. GOODRICH did not participate in any of the actual programmes, nor had he made any proposal for new programmes.

Date and Place of Next Meeting

Taking account of the wishes expressed by several members, in particular Prof. A. S. LODGE, it was decided to hold the next meeting in Paris on 19-20 June 1975. That meeting would be devoted exclusively to rheology: the programme on SBS block copolymers, discussion of results obtained in the LDPE and PVC programmes (MEISSNER, WALES, LODGE) and proposals for new programmes: PVC (CHAUFFOUREAUX), branched elastomers (BÖHM)

M. CARREGA

IUPAC COLLEAGUES DECEASED

We have been informed of the death of:

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|------------------------------------|---|
| <i>Belgium</i> | Dr. P. R. L. A. DALQ (21 December 1974)—Section on Water Quality (1969-1975) |
| <i>Federal Republic of Germany</i> | Prof. TH. FÖRSTER (20 May 1974)—Physical Chemistry Division Committee (1965-1969), Commission on Molecular Structure and Spectroscopy (1963-1973), Sub-Commission on Ultraviolet Spectroscopy (1963-1967)

Prof. H. REMY (27 November 1974)—Commission on Nomenclature of Inorganic Chemistry (1955-1971), Commission on Atomic Weights (1959-1967) |
| <i>UK</i> | Sir ROBERT ROBINSON (8 February 1975)—Vice-President (1936-1947), Bureau (1947-1951), Organic Chemistry Division Committee (1951-1955) |
| <i>USA</i> | Prof. E. R. LIPPINCOTT (24 December 1974)—Commission on Molecular Structure and Spectroscopy (1969-), Sub-Commission on Infrared and Raman Spectroscopy (1967-1971) |

REPORTS OF IUPAC-SPONSORED SYMPOSIA

IX INTERNATIONAL SYMPOSIUM ON CHEMISTRY OF NATURAL PRODUCTS

Ottawa, 23-28 June 1974

Around 750 scientists and 200 accompanying persons registered for this meeting at Carleton University campus, Ottawa. About 25% of these came from overseas, and around 50% from USA. Nearly 500 of the scientist registrants stayed in residence at Carleton University, thus leading to a very compact meeting. Many registrants expressed appreciation of the togetherness, in contrast to conferences in larger centres where the unavoidable use of many hotels leads to a more diffuse group. The social programme was also arranged to encourage intermingling of the participants.

The Organizing Committee experimented (successfully according to many comments) with a somewhat different programme arrangement than hitherto tried at Natural Products Symposia. Firstly, the subject divisions were chosen with emphasis on rapidly developing areas (e.g., Insect and Marine Chemistry, Bioorganic Chemistry) and peripheral areas (Natural Products of Medicinal Interest), as well as more traditional groupings (Synthesis, Structure and Properties, Transformations of Natural Products). Secondly, besides the introductory lecture by Prof. C. DJERASSI and an array of one-hour featured speakers covering all areas [to be published in *Pure and Applied Chemistry* in 1975 (scheduled Vol. 41, Nos. 1-2)], over forty other outstanding workers were asked to present special half-hour lectures. The latter were offered no financial help to attend beyond waiver of registration fees, but the opportunity to present the longer lecture led to nearly complete acceptance of the invitations. Thus, at little extra cost, the Symposium was able to expose the participants to 40 half-hour lectures of very high quality. These speakers and the one-hour ones had not been featured at either of the last two IUPAC Natural Products meetings. While some overlap in time of these featured lectures was unavoidable, it was kept to a minimum, and where possible the overlapping talks were in widely different subject areas.

The quality of the 193 contributed papers was high. Of these, 55 were on Synthesis and 52 on Structure and Properties, hence these more traditional areas are very much alive. Thanks to the large attendance and financial help from industry, National Research Council of Canada, Chemical Institute of Canada, IUPAC, and many universities, all expenses of the Symposium were covered.

C. T. BISHOP
O. E. EDWARDS

III INTERNATIONAL PESTICIDE CHEMISTRY CONGRESS

Otaniemi, 3-9 July 1974

His Excellency, the President of Finland, URHO K. KEKKONEN, had consented to act as Patron of the Congress, which was organized by the Federation of Finnish Chemical Industry. The Special Symposium on Dispersion Dynamics of Pollutants in Environment with Special Reference to Pesticides (5-6 July)

was organized by the Institute of Occupational Health (Helsinki) and the Institute of Ecological Chemistry of the Society for Radiation and Environmental Research Ltd. (Munich).

The following international organizations were represented by official delegates: EEC (Mme VAN DEN BRUEL-DORMAL and Mr. G. DEL BINO); FAO (Dr. E. E. TURTLE); IAEA (Dr. P. WINTERINGHAM); IUBS (Prof. N. OKER-BLOM); IUNS (Dr. A. AHLSTRÖM); IUPAC (Dr. D. C. ABBOTT); UNIDO (Mr. K. SZABO); and WHO (Dr. F. C. LU, Dr. J. W. WRIGHT, and Dr. V. KRICHAGIN). More than 1,000 scientists and 51 countries participated in the Congress. A total of 539 scientific papers was registered by the organizers, out of which about 450 were discussed in the Congress and the Special Symposium. The papers were given in 54 half-day sessions.

The scientific programme began with a Plenary Session of the following six invited speakers:

R. D. O'BRIEN (USA) spoke about 'The Design of Anticholinesterases'. The significance of new findings in two areas was discussed with respect to the design of inhibitors of acetylcholinesterase. One area was that of enzyme structure, including the oligomeric form, and the existence of allosteric binding sites, of isozymes, and of a mutant enzyme. The other area was that of the forces which bound inhibitors to the enzyme prior to their reacting with it: namely, ionic, hydrophobic, and charge-transfer bonds.

H. FREHSE (FRG) discussed 'Problems and Aspects of Present-day Residue Analysis'. A general picture was presented of the analytical, statistical, toxicological, and 'philosophical' role of pesticide residue analysis in the evaluation of food and environmental problems. The presentation was intended as an updating of the situation which was prevalent and described 3 years earlier, as well as an outlook on future trends and developments.

C. A. EDWARDS (UK) spoke about 'Factors that Affect the Persistence of Pesticides in Plants and Soils'. Some of the factors that influence the persistence of pesticides were common to both plants and soils. These were firstly, the characteristics of the pesticide, including its overall stability either as parent compound or metabolites, its volatility, solubility, formulation, and the method and site of application. A second group included the environmental factors, particularly temperature, precipitation, and air movement. Of these factors, the most important seemed to be related to the chemical stability and physical characteristics of the pesticide—its stability exerting the greatest influence, otherwise volatility being more important in soil and solubility in plants. Of the plant characteristics, the species and rate of growth seemed most important and in soil, adsorption to organic matter or clay minerals, and the populations of soil microorganisms present exerted the greatest influence.

K. MUNAKATA (Japan) presented a paper dealing with 'Insect Anti-feeding Substances in Plant Leaves'. He reported on the studies done with the leaves of various plants containing many kinds of antifeeding substances, *e.g.*, terpenes, alkaloids, and coumarins. The chemical structures had been resolved and the parent structure of the antifeeding substances was suggested.

L. I. MEDVED (USSR) spoke about 'Progress in Pesticide Toxicology in USSR'. He described the approach towards hygienic standards of pesticides in foods, working area air, atmosphere, and water. He also explored current research on the delayed effects of various pesticides on test animals.

E. KNÜSLI (Switzerland) discussed 'The Future of the Development of Pesticides by Industry'. The increased requirements for agricultural chemicals

had made the development of new products a most expensive operation, involving high industrial risks and low probability of success. In spite of these risks many companies were willing to accept the challenge. The activity of the companies depended, however, on local conditions, *e.g.*, operable regulations on the part of the legislator; an adequate system of production of technical goods; and the scrutiny and objectivity of the information media.

The scientific programme of the Congress comprised the following main topics:

1. Pesticide Residue Analysis
2. Pesticide Residues in Food and Feed Commodities and Total Diets
3. Impact of Environmental Factors on Chemical Behaviour of Pesticides in Plants, Soils, and Waters
4. Relationship of Chemical Structure to Biological Activity of Pesticides
5. Pesticide Metabolism
6. Pesticide Toxicology and Pharmacology
7. Chemistry and Activity of Naturally Occurring Pesticidal Compounds and Related Substances
8. Industrial Aspects of Pesticide Chemistry
9. Pesticide Legislation in Various Countries

The following symposia were organized under these main topics: Symposium 1A on Advances in Pesticide Residue Analysis Technology Including Automated Methods organized by K. R. HILL (USA). Symposium 1B on Mass Spectrometry in Analysis of Pesticides organized by S. SAFE (Canada) and O. HUTZINGER (FRG). Symposium 1C on Analytical Quality Control in Pesticide Residue Laboratories organized by K. A. McCULLY (Canada). Symposium 1D on Recent State of Residue Chemistry of Dithiocarbamates organized by R. ENGST (GDR). Symposium 1E on Instrumental and Bioassay Techniques for Analysis of Herbicide Residues organized by R. J. HANCE (UK). Symposium 3A on Effects of Environmental Factors on Pesticide Stability organized by A. AAPOLA (Finland). Symposium 3B on Conversion of Pesticides on Clay Surfaces organized by B. YARON (Israel). Symposium 4A on Recent Advances on Biodegradable Insecticides organized by G. T. BROOKS (UK) and J. J. MENN (USA). Symposium 4B on Adaptation Chemistry of Organisms to Pesticides organized by E. Y. SPENCER (Canada). Symposium 4D on Perspectives of Theoretical Fungicide Research organized by G. MATOLCSY (Hungary). Symposium 5A on Insect Microsomal Monooxygenases in Pesticide Metabolism organized by M. AGOSIN (USA). Symposium 5B on Mode of Action and Metabolism of Plant Growth Regulators organized by H. M. DEKHUIZEN (Netherlands). Symposium 6A on Dynamics and Toxicological Evaluation of Pesticide Loads in Animals and Man organized by H. G. VERSCHUUREN (Netherlands). Symposium 6B on Pesticide Exposure, Health Hazards, and Control Measures organized by F. C. LU (Switzerland). Symposium 7A on Chemistry, Biochemistry, and Insecticidal Action of Natural and Synthetic Pyrethroids organized by M. ELLIOTT (UK). Symposium 7C on Chemicals Affecting Insect Behaviour and Development organized by M. BEROZA (USA) and M. JACOBSON (USA). Symposium 7E on Chemosterilants for Controlling Insect Populations organized by A. B. BOŘKOVEC (USA). Symposium 8A on Enolphosphates—Synthesis, Properties, and Applications organized by S. FULDE (Poland). Symposium 9A on Pesticide Legislation in Various Countries organized by M. TOIVIAINEN (Finland).

The special Symposium on Dispersion Dynamics consisted of 16 invited lectures and a number of short communications. The invited lectures given were:

- H. FLOHN (FRG) 'Natural Longterm Changes of Global Environment'
- C. JUNGE (FRG) 'Transport Mechanisms for Pesticides in the Atmosphere'
- A. M. AITSAM (USSR) 'Transport Mechanism in Water'
- E. P. LICHTENSTEIN (USA) 'Transport Mechanism in Soil'
- L. I. MEDVED (USSR) 'Circulation of Pesticides in the Biosphere'
- P. BAGGE (Finland) 'Pesticide Residues in Some Baltic Animals: A Review of Selected Literature'
- M. GOTO (Japan) 'Pollution Problem of the Seto Inland Sea'
- L. ROSIVAL (Czechoslovakia) 'Ecochemistry of BHC in Czechoslovakia'
- J. ROBINSON (UK) 'Mathematical Models in Ecochemistry'
- C. L. DUNN (USA) 'The Value of World-wide Pesticide Residue Monitoring Systems'
- M. WASSERMANN (Israel) 'Organochlorine Compounds in the General Population of the 70's and Some of Their Biological Effects (in Man and Animals)'
- F. COULSTON (USA) 'Mutagenic, Carcinogenic, and Teratogenic Effects of Pollutants in Respect to Man'
- J. CLAUSEN (Denmark) 'The Content of Polychlorinated Hydrocarbons in Arctic Animals'
- D. G. CROSBY (USA) 'The Toxicant-Wildlife Complex'
- A. KAMIŃSKI (Poland) 'Use of Biological Tests for Examination of Pesticides—I'
- E. E. KENAGA (USA) 'Use of Biological Tests for Evaluation of Pesticides—II'

At the conclusion of the Congress, four discussion sessions were held with the purpose of summarizing the results of the discussions and outlining the important areas of interest for future research.

Discussion session on Methodology for Analysis of Pesticides, Chairman—K. R. HILL (USA). Members of the panel: A. AMBRUS (Hungary), V. BÁTORA (Czechoslovakia), H. FREHSE (FRG), R. GREENHALGH (Canada), J. MIYAMOTO (Japan), and G. WIDMARK (Sweden). In his report, the Chairman of the discussion group stated that the field of residue analysis was becoming increasingly concerned with compounds containing nitrogen, oxygen, or sulfur atoms which required more sophisticated approaches and equipment. A concern about polar metabolites, usually lipid insoluble, was expressed; but the residue analyst needed to learn the significance of these residues from the toxicologist before expending increased effort and expense on developing the needed analytical methods. Also, the panel felt that more collaborative studies were needed to substantiate published methods of analysis. The cleanup process was continuously felt to be the one with the most challenging problems. More research was needed on methods such as gel permeation chromatography, sweep codistillation, *etc.*

Discussion session on Methodology for Design of New Pesticides, Chairman—E. KNÜSLI (Switzerland). Members of the panel: J. BASKAKOV (USSR), M. ELLIOT (UK), G. KEMPTER (GDR), G. MATOLCSY (Hungary), S. MATSUNAKA (Japan), and G. J. M. VAN DER KERK (Netherlands). The panel felt that the design of new pesticides required a group of scientists, including biologists, biochemists, analytical chemists, *etc.* New substances could be searched for along the following lines: looking for molecular variations of known substances with known biological activities; synthesizing new sub-

stances along routes based on known biochemical evidence of the target organism; identifying and elucidating new chemicals which were purposely looked for or which were accidentally observed to have biological activity; and screening of as many chemicals on as many targets as possible. It was stated that the biological activity of a compound was usually the first thing to look for, but the activity had to be judged in the light of other parameters like selectivity, environmental behaviour, toxicology, etc.

Discussion session on Methodology for Evaluation of the Impact of Pesticidal Compounds on the Environment, Chairman—F. KORTE (FRG). Members of the panel: P. WINTERINGHAM (Austria), E. E. KENAGA (USA), A. VOPIO (Finland), R. HANSON (USA), R. ENGST (GDR), R. KLJAJIĆ (Yugoslavia), and E. MRAK (USA). The panel recommended that a commission should be established as soon as possible to examine and discuss the terminology currently used in environmental research. The panel felt that the tendency of separating environmental problems into categories such as air, water, and soil, should be avoided because it had now been established that, in most cases, chemicals were being degraded and returned to the biosphere. The group felt the need of establishing a worldwide plant, animal, and human tissue analysis programme. In such a programme the trends of increase or decrease of chemicals in tissues could be followed. An important feature of the programme would be the storage of tissues to give scientists the opportunity of studying tissues of previous time periods. In its report the group also put forth a request for worldwide production figures and use patterns of pesticides.

Discussion session on Methodology for Evaluation of Safety of Pesticides to Man, Chairman—R. TRUHOUT (France). Members of the panel: J. I. KUNDIEV (USSR), L. ROSIVAL (Czechoslovakia), F. C. LU (Switzerland), W. F. ALMEIDA (Brazil), H. G. VERSCHUUREN (Netherlands), S. D. MURPHY (USA), and F. KALOYANOVA (Bulgaria). The panel agreed with the general conclusion of the WHO Scientific Group on Carcinogenicity and Mutagenicity that thresholds could be envisaged for carcinogens but stressed that, before establishing thresholds, there was a great need for adequate quantitative studies, especially at low levels. The problem of possible potentiation of toxic effects of pesticides as a result of association with other environmental pollutants or factors, such as noise and high temperatures, was recognized as important for research in toxicological evaluation. The criteria for selecting the most suitable species for extrapolation to man were examined critically. Reference was made to the use of some special animal species and to the significance of liver cell tumours in mouse. Several criteria for toxicological evaluation of pesticides were discussed: inhibition of cholinesterases and carboxyesterases in the case of organophosphorus insecticides; enzymatic inductions; pharmacokinetic studies; and modifications of conditioned reflexes. Reference was made to reliance on comparative biochemical findings in man and laboratory animals for prediction of longterm toxic effects in man. Also, the influence of the composition of the diet, especially the level of proteins, on the results of experimental feeding studies was discussed.

Plenary lectures and the invited lectures of the special Symposium will be published in the IUPAC Journal *Pure and Applied Chemistry* during 1975 (scheduled Vol. 42, Nos. 1-2). Other papers will be considered for publication by: *Environmental Quality and Safety*, *Residue Reviews*, *Archives of Environmental Contamination and Toxicology*, *Bulletin of Environmental Contamination and Toxicology*, and *Kemia-Kemi*. No special congress publication is planned. Information on the publication programme is available from the

Federation of Finnish Chemical Industry (POB 13028, SF-00131 Helsinki 13, Finland).

It is intended to hold the IV International Congress of Pesticide Chemistry in Basle during 1978.

J. KOIVURINTA and P. VARO

INTERNATIONAL SYMPOSIUM ON MACROMOLECULES

Rio de Janeiro, 26-31 July 1974

The Symposium was held under the sponsorship of IUPAC, Brazilian Academy of Sciences, Brazilian National Research Council, and Secretariat of Science and Technology of the State of Guanabara. Its aims were to contribute to the transfer of the newest macromolecular research results and to provide a forum for informal discussion. This was the first IUPAC meeting on macromolecules to be held in Latin America. In keeping with the high standards of the previous symposia on this subject, many of the speakers were of international reputation. The registration was over 700 people, from 25 countries. This included about 550 active participants, with about 50% coming from Brazil. A large number of Brazilian students from all parts of the country were attracted by the Symposium, holding promise for the future of macromolecular research in Brazil.

The programme was divided into four parallel sections:

- Section A — Polymer Chemistry
- Section B — Polymer Physical Chemistry
- Section C — Polymer Technology
- Section D — Biopolymers.

The 7 sessions of each section were composed of a single main lecture (45 minutes in length) and an average of 6 contributed papers (each 20 minutes in length). The main lectures, scheduled to have a minimum of overlap between sessions, are being published by Elsevier Scientific Publishing Co. in a special volume.

All abstracts of contributed papers were published in a paperback volume, *Contributed Papers—Abstracts*. During the sessions a discussion period was held for each of these contributed works. An effort was made to record the discussions and put them into print in the form of questions and answers on Discussion Cards. On the closing day of the Symposium, the booklet *Contributed Papers—Discussion* was available to all participants. Copies of both booklets can still be obtained from Academia Brasileira de Ciências, C.P. 229, 20.000 Rio de Janeiro, Brazil.

During the Opening Session, Prof. CARL S. MARVEL was honoured for his outstanding contributions to the development of polymer research in the world. Sir HARRY MELVILLE (University of London) presented the opening plenary lecture 'Trends in Polymer Science'. The closing plenary lecture, 'Polymers Worldwide: Review and Preview', was given by Prof. H. MARK (Polytechnic Institute of New York).

In Section A—Polymer Chemistry, Session A-1, C. G. OVERBERGER (University of Michigan) reported in a main lecture about the 'Reactivity of Polymers in Organic Reactions'. The topics of the contributed papers of that Session varied from polymeric reactions and reactions on polymers to polymerization in interacting systems.

In Session A-2, M. FARINA (University of Milan) reported his results on 'Inclusion Polymerization', whereby emphasis was placed on the preparation of optically active polymers included in the channels of optically active perhydrotriphenylene. The contributed papers were concerned with charge transfer polymerization. One paper discussed the possibility of preparation of polymers with phthalocyanine, hemiporphyrizine, and porphine.

Session A-3 opened with 'Photopolymerization and Photoresponsive Polymers' by G. SMETS (University of Louvain), pertaining to polymer systems crosslinked by irradiation in dependence of the state of aggregation and the temperature. The report included the morphology, adhesive properties, and solubility of crosslinked and noncrosslinked areas of polymer films during irradiation. The contributed communications were concerned with photopolymerization of EDA complexes, photografting from the vapour phase, plasma polymerization of saturated hydrocarbons, as well as the polymerization of *N*-fluorophenylmaleimides.

H. RINGSDORF (University of Mainz) reported in Session A-4 on 'Structure and Properties of Pharmacologically Active Polymers', while in one contributed paper the potential use of polymeric sulfadiazine as carrier for an anticancer agent was discussed. Other papers treated the anionic polymerization of α -methylstyrene and ethylene oxide, the synthesis of *p*-benzoquinone homopolymers and *p*-benzoquinone-styrene cooligomers by cationic initiation.

Session A-5 started with the main lecture of G. B. BUTLER (University of Florida), 'Perspectives in Cyclopolymerization'. This presented the still remaining conflicting aspects of the cyclization step by discussing the experimental evidence, *e.g.*, bathochromic shifts of the monomer, activation energy, degree and rate of polymerization, ring size, and volume contraction on cyclopolymerization. The synthesis and properties of high molecular weight poly (organophosphenes) as one of the few successful attempts to prepare useful inorganic polymers, and the conditions for polymerization of olefins in liquid sulfur dioxide to yield homopolymers, polysulfurs, and mixtures thereof, were the subjects of contributed papers. Furthermore, the membrane properties of polymers with pendant phosphonate groups were also discussed.

L. PORRI (Polytechnic Institute of Milan) in Session A-6 gave a survey of 'Polymerization of Conjugated Diolefins by Transition Metal Catalysts: Recent Developments', placing emphasis on the still controversial mechanism of insertion and its connection with the resulting polymer microstructure, as well as on new catalysts and polymers of commercial interest. The communications in this Session covered a variety of subjects, such as the microstructure of polyalkyl- α -chloroacrylates dependence on polymerization conditions, general aspects of the control of cationic vinyl polymerization on the basis of EDA complexation, and a study of the formation of cobalt, nickel, and iron complexes with polyvinylpyridine and polyvinylpyrrolidone.

In the closing session of Section A, J. K. STILLE (University of Iowa) reported about the research of his group on 'Synthesis of Rigid Chain Polymers' by $4 + 2$ cycloaddition and the Friedlander reaction, stressing the preparation of soluble products by appropriate phenyl substitution. Two contributed communications dealt with polymerization in ordered media, *i.e.*, polymerization in nematic phases and solid state polymerization of 4-vinylpyridinium salts. A related subject was the determination of transfer constants for polymerization of styrene in the presence of low molecular

weight styrenes. A novel, semiconducting and thermally stable polymer was prepared by polycondensation of 1-acenaphthenone.

In Section B—Polymer Physical Chemistry, the main lecture of the first session was 'On the Effect of Internal Concentration on Some Properties of Polymer Solutions' by H. BENOÎT (Research Center on Macromolecules, Strasbourg). One contributed paper of this Session dealt with the inadequate treatment of polymer solutions by current theories in the light of experimental findings of polystyrenes of extremely high molecular weight. Conformational transitions of polymethacrylic esters by changing the composition of binary solvent mixtures was discussed. Other papers dealt with the general treatment of chirality in vinyl polymers without asymmetric side groups, and with the semiconductor properties of polyconjugated polymers obtained by a Wittig reaction.

The main lecture of Session B-2 by S. KRIMM (University of Michigan), 'Infrared Studies of Chain Organization in Crystalline Polyethylene', used the theory of crystal infrared spectroscopy and specific deuteration to elucidate the nature of folding in polyethylene single crystal. The communications ranged from determination of the dichroic ratio, in polarized IR radiation to determine the orientation distribution in stretched films, neutron scattering of deuterated polymers in an undeuterated matrix, a general method for estimation of the heat of polymerization by vibrational stretching frequencies and the potential of Laser-Raman spectroscopy in polymers, to the pyrolysis and fragmentation of polybenzyls in an electron impact mass spectrometer.

P. MEARES (University of Aberdeen) in Session B-3 gave a concise review of 'Selective Transport Processes in Polymers', discussing diffusive, convective, and 'facilitated' transport mechanisms in membranes, *e.g.*, in gel membranes, hyper filtration, electrodialysis, and membrane electrodes. Contributed papers were concerned with glass transitions in ethyl acrylate monomers, drag reduction in polymer solutions, and absolute particle size distributions from disc centrifuge photodensitometer data.

M. SZWARC (University of Syracuse) reviewed 'Anionic Polymerization: Its Past Achievements and its Present Status' in Session B-4. Special attention was devoted to the synthesis of block copolymers and their unusual solution properties and zwitterions. During this session a study of interpenetrating polymer networks, prepared by curing preformed mixtures of prepolymers, and their mechanical properties was presented. Also presented was a study of the dependence of electric birefringence and electric dichroism of polyelectrolytes on concentration and ionic strength as well as the effect of polyelectrolytes on the kinetics of reactions with ionic species.

In Session B-5 a main lecture on 'Determination of MW Distribution by Column Methods and the Relations between the Distributions and the Mechanism of Polyreactions', was presented by G. V. SCHULZ (University of Mainz). This treated theoretical and methodical aspects of the presently available chromatographic systems for polymers and the interrelations of the results with the microstructure. Short communications covered universal calibration curves as extended to oligomers whose sequential distribution was nonGaussian, increase in theoretical plates and decrease in analysis time by using small diameter porous gels in GPC, and a statistical-thermodynamic treatment of the efficiency of precipitation fractionation in columns. Also discussed were the molecular weight distributions of polydisperse homopolymers obtained from gel chromatography as compared with the most commonly used theoretical distribution functions, the relation between

preferential absorption in binary solvent mixtures and the refractive index increment, and finally the determination of binodal edges of precipitation of polymer from binary solvent mixtures.

Session B-6 featured as the main lecture 'High Resolution Carbon-13 Studies of Polymer Structure' by F. A. BOVEY (Bell Laboratories, USA). Emphasis was placed on a general gauche CH...CH interaction model to explain the chemical shift of the carbon-13 spectra and its application to elucidate the nature of the branches in polyethylene and polyvinylchloride. The majority of the papers of this Session were reports on the NMR spectra of homo- and copolymers, *e.g.*, stereoregularity of a variety of vinyl polymers as elucidated by carbon-13 resonance, evaluation of sequence probabilities by joint application of carbon-13 and proton resonance in different NMR solvents, and tacticity of polypropylenesulfide using paramagnetic shift reagents. Furthermore, a calculation method for the evaluation of different species of ion pairs in ionic solution polymerizations, based on conductivity measurements, was presented.

The main lecture of the closing session of Section B, 'The Role of Molecular Mobility in Polymer Photochemistry', was presented by J. GUILLET (University of Toronto). Examples of the influence of rotational and translational processes in polymeric ketones were given in connection with solid-state phase transitions and also on the effect of diffusional mobility of oxygen in polymers influencing the quenching efficiency. Other topics of this Session centred on the solid state of polymers. Thus, a theory of crystal thickening during annealing, based on irreversible thermodynamics, was presented as well as a theory on the crystallization of polymers in flat crystals with ordered refolding. More experimentally oriented papers were connected with the crystallization during polymerization of monomers, crystallization of polyethyleneoxide in AB block copolymers, and the use of covalently attached spin probes to elucidate the molecular motion as compared to NMR, dielectric, and T_g determination of molecular motion.

In the main lecture in Section C—Polymer Technology, Session C-1, B. RÅNBY (Royal Institute of Technology, Stockholm) presented his views on 'Creativity in Teaching and Research in Polymer Technology'. His ideas raised interesting debates on the topic. Other papers dealt with theoretical aspects of mastication of polyethylene, molecular architecture in anionic polymerization of diene elastomers, electron conductivity of plasticized polyvinylchloride compositions, application of group theory concepts to describe adequately differently organized copolymer architectures, reproducibility of particle size within a narrow range of diameters in suspension polymerization, and measurement of viscoelastic properties.

In Session C-2, the main lecture reported on 'Advances in Polyethylene Technology', and was presented by F. C. FOSTER (Chemplex Company, USA), attention being given to synthesis variables which determine the polymer structure in low and high density polyethylenes. Short contributions treated the effects of cold extrusion on polyethylene, the meaning of accelerated ageing test for polymers, and the influence of oxygen in the suspension polymerization of vinyl chloride.

'Pyrolysis and Fine Structure of Cellulose' was the subject presented by M. LEWIN (Hebrew University of Jerusalem) in Session C-3. Emphasis was given to the increase in the rate of pyrolysis by an increase of the percentage of low ordered regions (LOR). Contributed papers in this session were related to natural industrial macromolecules. Humic acid fractionation, organization of cellulose and amylose triacetates in monomolecular films at aqueous inter-

faces, structural relationship between the humins of mineral coals and phenolic resins studied through thermogravimetry, and conversion of coal to different products of commercial interest by chemical reactions (like liquid phase oxidation, depolymerization with hydrogen or halogens, sulfonation, and ammoniation). Furthermore, a theory involving heterogeneous depolymerization kinetics was presented which permits the use of simple kinetic experiments as a probe for a study of structure of insoluble polymers. An evaluation of the xanthate reduction method for grafting of acrylonitrile onto wood pulp was discussed. The use of ultrasound to generate free radicals in a continuous flow reactor in order to increase the rate of chemically initiated vinyl polymerization was also reported.

Session C-4 had as the principal topic 'Some Advances in Synthetic Fibre Technology', presented by S. OKAMURA (Kyoto University). The manufacture and properties of polyvinylchloride fibres from the polymer emulsion by direct spinning were discussed. Papers in this Session dealt with the application of grafted solid surfaces of polymers as sorption agents for pollution control, thermal shrinkage exhibited by cold-drawn aromatic polymer films (which was related to the local molecular relaxations of the chain units), plastic deformation of fibrous structures, conversion of crosslinked phenol-formaldehyde fibres in new fibres by reactions like chemical blocking of the phenolic hydroxyl, oxidation of the methylene bridge, and sulfonation and methylation of the aromatic ring, and adhesive bonding of wool by acrylonitrile-butadiene copolymers which could be crosslinked between the wool components to give high adhesive strength.

I. V. YANNAS (Massachusetts Institute of Technology) reported in Session C-5 on 'Molecular Interpretation of Deformation in Glassy Polymers'. Using a glassy polycarbonate as the model polymer, the author showed that a three-bond chain segment, whose rotation around the centre bond was hindered primarily by intermolecular forces, could account at the molecular level for much of the mechanical behaviour of that polymer. He suggested that the three-link chain backbone segment, interacting according to a Lennard-Jones potential with its nearest neighbour during rotation around its central link, might provide a satisfactory preliminary basis for a molecular interpretation, extendable to glassy polymers in general. Contributed papers in this Session discussed measurement of bond stresses in polymers subjected to strain by the shift in peak position and change in shape of infrared absorptions, quantitative description of a polymer structure which depended on thermomechanical history by the relative amounts of enthalpy and entropy, effects of terminal chains on the dynamic mechanical properties of block copolymer blends, damping and noise attenuation of interpenetrating polymer networks, characterization of lubricants for polyvinylchloride, and prediction of hysteresis for nonlinearly viscoelastic materials through equations.

Scientific and technological aspects of 'Advances in Synthetic Rubber', were reviewed by M. MORTON (University of Akron), who emphasized recent developments in the control of average molecular weight in free radical polymerization, control of chain unit structure, control of molecular weight distribution, block copolymers and thermoplastic elastomers, and liquid rubber technology. Still in Session C-6, elastomer structure and composition were discussed in short papers, which considered elastic and visco-elastic properties, effect of pressure on mechanical behaviour, influence of humidity and oxygen in long-time creep, and sulfur vulcanization of natural rubber.

Interpenetrating polymer networks were also reported for an incompatible and for a semicompatible polymer pair.

The last session of Polymer Technology, Session C-7, presented as the main lecture 'Copolycondensation: Relationship between Structure and Properties in New Polymers of High Thermal Stability', by J. FONTÁN (Institute of Plastics and Rubber, Madrid). Special attention was given to copolyimides in which groups including ester, amide, anhydride, epoxy, titanate, as well as heterocyclic rings, were present in the chemical units. Papers dealt with diversified technological subjects. Polybenzimidazole degradation studies, flame retardant monofilaments spun from molten polyethyleneterephthalate systems, miniature strip specimens prepared in the laboratory from cast films for tensile evaluation of small amounts of polymer samples, a mathematical model for determination of kinetic parameters in the industrial preesterification of dimethyl terephthalate with ethylene glycol, and high impact new polyesters as engineering materials, were discussed.

Section D—Biopolymers, Session D-1, featured ^1H and ^{13}C NMR Studies on Carbohydrate Polymers: Structure of Mucopolysaccharide' by A. S. PERLIN (McGill University), stressing the study of mucopolysaccharides. Proton NMR investigation of heparin led to a revised structure for that biopolymer. The carbon-13 investigation was based on comparison with model compounds and included spin relaxation measurements. Contributed papers of this opening Session presented results on the bacterial synthesis of cellulose, observing a parallelism between chain growth and bacterial population growth. Furthermore, the viscosity data of cellulose and amylose tricarbanilates were used to draw conclusions on coiling in solution, the 2-cyclohexyloxy-tetrahydropyran derivatives were used as model compounds for polyglucosidic sequences to study their intramolecular hydrogen bonding, electrochemical properties of membranes of grafted cellulose were measured as a function of electrolyte concentration, and nonNewtonian behaviour of cellulose solutions was investigated.

In Session D-2, E. DE ROBERTIS (University of Buenos Aires) reported his results on 'Isolation and Molecular Properties of Receptor Proteins for Neuroactive Drugs'. The receptors were isolated by conventional and affinity chromatography and their interaction with drugs was studied by light scattering, fluorescence, electron microscopy, and X-ray diffraction, finding for some receptors an ordering into paracrystalline arrays. The other papers of this Session included a combined ESR and UV study of the micellar structure of detergents, a UV-CD study on the conformation of polypeptides of lipid matrices held in suspension, an ORD investigation of crotamine in dependence of pH and denaturation, and a spin label study of the hormone angiotensin in interaction with smooth muscle membrane.

H. G. KHORANA (Massachusetts Institute of Technology) presented a main lecture in Session D-3 on 'A Bacterial Gene for Tyrosine Transfer RNA: Promoter and Terminator Sequences and Progress in Total Synthesis'. The report included the total synthesis of the double-stranded DNA corresponding to the full length of the terminator region of the gene, total synthesis of the promoter and terminator regions with appropriate single-stranded protruding ends for later joining, end to end joining of the various synthetic parts of the gene to form the total gene, controlled transcription of the synthetic gene, and stepwise processing of the RNA product to produce biologically functional tRNA. The papers of this Session were concerned with preparative aspects as well as physical characterization, *e.g.*, synthesis of

oligonucleotides on polymer supports, cooligocondensation of nucleic acid constituents, independent transcription of 16 S and 23 S r-RNA in *Bacillus subtilis*, translation from Ehrlich ascites tumor cells in a cell free system, and helix-coil transition in nucleoprotein.

In Session D-4 'Reactive Polymer Carriers and the Immobilization of Enzymes' was the topic of G. MANECKE (University of Berlin). Different possibilities for immobilization and the change in the properties of the enzyme by immobilization were treated. Some subjects of the contributed papers were the kinetic behaviour of enzymes entrapped in gels by microspectrophotometric techniques observing the inner portion of a gel particle, a study of the active site of rat liver RNA by the use of inhibitors and the pH dependence of activity, chemical protection by N- and S-containing polymers against γ -radiation, and a binding study on β -trypsin.

R. B. MERRIFIELD (Rockefeller University) reported on 'Synthetic Approaches to the Study of Proteins' in Session D-5. The semisynthetic enzyme formed by covalent bonding of the synthetic C-terminal tetradecapeptide of ribonuclease with a shortened protein component, RNase 1-118, was used to examine the role of several amino acid residues in the functioning of ribonuclease. Replacement analogues of His¹¹⁹, Phe¹²⁰, Asp¹²¹, Ser¹²³, and Val¹²⁴, were synthesized and the complexes formed with RNase 1-118 were tested for enzymatic activity. Short communications of the Session dealt with polypeptatides as polypeptide models for helix-coil transitions, theory of helix-coil transitions of polypeptides based on a three state Ising model, theory of unzipping of polynucleotides by making assumptions about the different rate constants, and studies on the conformation and preparative aspects of polypeptides.

'Role and Regulation of Poly- β -hydroxybutyrate as a Reserve in Microorganisms' by E. A. DAWES (University of Hull), treated in Session D-6 the functioning of this polymer as an energy reserve, investigating also the conditions for accumulation in microorganisms and the enzymology of synthesis and degradation. Further topics in the Session were concerned with a quantitative model for the effect of binary solvent compositions on conformational transitions of different types in polypeptides, preparation of butadiene-peptide AB block copolymers which formed liquid crystalline structures in solution, and a contribution to the polymerization of NCA by an 'activated monomer' mechanism.

In the closing Session of Section D, H. G. PEREIRA (Animal Virus Research Institute, UK) summarized the 'Polymerization of Adenovirus Proteins', by studying the different polymeric states of these proteins by crystallography, electron microscopy, and analytical centrifugation, relating structure studies to the polymerization of the proteins. The contributed papers included the mathematical treatment of the formation of macromolecules like cellulose as controlled by the growth of the bacterial cells, ORD for studying the interaction of quaternary ammonium compounds with natural polyelectrolytes, and the enzymatic specificity of the enzyme kallikrein.

This Symposium was made possible mainly by funds given by the Brazilian Government through the following agencies: Academia Brasileira de Ciências, Conselho Nacional de Pesquisas, Secretaria de Ciência e Tecnologia do Estado da Guanabara, Coordenação de Aperfeiçoamento do Pessoal de Nível Superior, Centro para a Aplicação da Ciência e da Tecnologia ao Desenvolvimento da América Latina, Conselho Federal de Química, Divisão de Ciência e Tecnologia do Ministério das Relações Exteriores, and Organização de American States.

E. B. MANO

VII INTERNATIONAL SYMPOSIUM ON CARBOHYDRATE CHEMISTRY

Bratislava, 5-9 August 1974

The Symposium was organized by the Bratislava Institute of Chemistry of the Slovak Academy of Sciences under the sponsorship of IUPAC. Held at the Faculty of Engineering of the Slovak Technical University in Bratislava, the meeting was attended by about 420 participants from 27 countries (320 from abroad). It was opened by Dr. ŠTEFAN BAUER, Director of the Institute of Chemistry. At the Opening Ceremony, Dr. M. REPÁŠ (Secretary General of the Slovak Academy of Sciences) spoke on behalf of the Honorary Board. He welcomed the participants and analyzed the influence of science on civilization and the importance of international scientific cooperation. Prof. R. WHISTLER spoke on behalf of the International Steering Committee for Carbohydrate Chemistry. A pleasant event at the Opening Ceremony was the presentation of an Honorary Issue of the journal *Carbohydrate Research* to one of the most distinguished carbohydrate chemists, Prof. H. ISBELL, dedicated to him on the occasion of his 70th birthday. The presentation was performed by Prof. J. M. WEBBER.

The programme covered three main topics: general organic chemistry of saccharides and their derivatives; chemistry and biochemistry of plant and wood polysaccharides; and biochemistry of carbohydrates in general, with the emphasis on polysaccharides and related biopolymers, their structure and biological activities. Because all these fields overlap particularly in view of final goals and experimental methods, the Organizers reserved each morning for plenary lectures from the above areas of carbohydrate chemistry and biochemistry, which were presented by invited speakers who had gained an international reputation in their respective fields.

Prof. D. HORTON presented an excellent account of work done on the synthesis of thiosugars and their use in carbohydrate synthesis as starting materials for various sugar derivatives. Use of modern physicochemical methods led to the final resolution of the stereochemistry of 2-thiosugars and some acyclic sulfur-containing sugar derivatives. Several acyclic thiosugar precursors were used for the synthesis of nucleoside antimetabolites of various stereochemistries and conformations. Some of the prepared derivatives exhibited significant antitumour activity; this was found to be dependent on the stereochemistry of the acyclic carbohydrate chain.

Prof. W. G. OVEREND discussed recent developments in the chemistry and synthesis of unusual aminosugars and branched chain sugars. He presented new elegant routes for preparation of this type of derivative.

Prof. N. K. KOCHETKOV reviewed the methods for chemical synthesis of polysaccharides. His group had elaborated synthetic procedures based on two basic principles: synthesis from monomeric precursors and synthesis from oligosaccharide precursors. He presented examples of different approaches for the synthesis of products with desired structure.

Prof. YU. S. OVODOV gave a brief review of structural features of all plant polysaccharides containing glycuronic acid residues so far identified in nature. He attempted to classify this group of natural substances on the basis of the structure of their basic core. He also critically evaluated the present stage of research on acidic plant polysaccharides. Furthermore, he issued a challenge to study more the biological activities and physiological functions of these substances in plants, and their interaction with other cell wall components.

The plenary lecture of Dr. R. KOHN was concerned with the latest achievements on interaction of bivalent cations with the carbonyl groups of polymers. Comparison of ion binding on polygalacturonate, polymannuronate, and polyglucuronate, and on partially esterified polygalacturonic acids, led to the conclusion that cation binding on polyuronates was dependant not only on the linear charge density of macromolecules but also on their conformations. He also presented clear evidence for the existence of intermolecular binding of bivalent cations, which was the most important factor influencing cation exchange reaction.

Prof. R. H. MARCHESSAULT pointed out that the assessment of crystal structures of polysaccharides, based on the crystal structures of free and of peracetylated oligomers, should be conducted on only identically related oligomers. A comparison of the crystal structures of free and peracetylated hexapyranose disaccharides showed marked differences in torsional angles around skeletal and glycosidic bonds. The effect of acetate substitution was not so appreciable for pentopyranose disaccharides.

The significance of immunochemical approaches in structural studies of polysaccharides was discussed by Prof. C. V. N. RAO. He presented numerous examples of how cross reaction with specific antisera led to the discovery of new structural features in polysaccharides. He pointed also to the limitations of immunochemical methods in the case of sugar residues having similar conformations. The general feeling was, however, that the number of papers from this field had been decreasing in recent years, due to the application of more powerful physicochemical methods for elucidation of polysaccharide structure.

Recent progress in the biochemistry of bacterial cell walls was the subject of the plenary lecture by Prof. J. BADDILEY. The emphasis in his talk was directed particularly to regulation of biosynthesis of two basic wall components of Gram-positive bacteria, peptidoglycan and teichoic acid. Both these components utilized undecaprenol monophosphate as a common lipid intermediate for their biosynthesis, an interesting feature which might serve as a regulatory factor of the overall rate of both biosynthetic pathways. It had also been shown that a number of control steps occurred in the synthesis of nucleotide sugar precursors of one wall component by nucleotide precursors of the other component. Evidence was presented for the presence in the bacterial membrane of a phosphorylated glycoprotein of so far unknown biological function.

Prof. J. MONTREUIL surveyed the structures of various animal glycoproteins. By means of four basic methods of degradation of carbohydrate chains (mild acid hydrolysis, acetolysis, hydrazinolysis, and enzymic hydrolysis), he established the main structural features of carbohydrate chains, and by comparing these basic features of various glycoproteins came to the conclusion that there was essentially no diversity in the basic plan of this group of biologically important substances.

The contributed papers fitted essentially into the outlined scope of the Symposium programme. They were presented in the afternoon sessions. In the organic chemistry sessions one observed that extensive work had been done on preparation of a large number of new carbohydrates and their derivatives. The standard of synthetic procedures corresponded to the present stage of carbohydrate chemistry. Many of the new compounds and reactions would certainly find their application in carbohydrate syntheses, and the antimetabolites and aminoglycoside antibiotics would be useful in biological

research and medicine. A considerable part of the contributions was devoted to fundamental physicochemical methods, such as NMR, mass spectroscopy, and chiroptical methods. The participants witnessed for the first time, examples of the use of nitrogen-15 NMR spectroscopy in structure elucidation of aminosugars (COXON). Only slight attention was devoted at the Symposium to electrochemical transformation of sugars and to reaction kinetics.

In sessions devoted to plant and wood polysaccharides, the contribution of KUNIAK attracted attention, dealing with possibilities of large application of crosslinked polysaccharides in biochemistry and medicine and use of cross-linking itself for preparation of hydroxyethylcellulose fibres. Structural features of various polysaccharides was a common theme. One felt in each contribution of this type, that this branch of carbohydrate chemistry had gained in recent years from modern physicochemical methods which were powerful tools in elucidation of structures and conformations of polysaccharides. Other important contributions were those dealing with specifically directed degradation of polysaccharides, particularly these concerned with the more complex structures of heteropolysaccharides (ASPINALL, LINDBERG, and their school).

A large number of contributed papers were devoted to the biochemical aspects of carbohydrates. They could be divided into two basic groups: those dealing with structure and biological properties of microbial polysaccharides, animal glycoproteins and their constituents; and those dealing with biosynthesis and enzymic degradation of polysaccharides. One recalls the paper describing unusual constituents of microbial lipopolysaccharides (LINDBERG) and the new discovery of a structurally interesting 'inner core' of yeast mannan and elucidation of the point of its attachments to protein, analogous to bacterial and animal antigens (BALLOU). There is, however, no space to quote here other excellent contributions. As far as possible, the Organizers tried to arrange the submitted papers into more or less monothematic sessions, which contributed much to lively discussions of individual papers. Abstracts of all submitted contributions were published whether they were presented on the platform or not, and these can still be purchased from the Organizers (Institute of Chemistry, Slovak Academy of Sciences, Dúbrowská Cesta, CS-809 33 Bratislava, Czechoslovakia).

In keeping up with general policy of all IUPAC meetings, the plenary lectures presented will be published in *Pure and Applied Chemistry* (scheduled Vol. 42, No. 3, 1975) and will also be available as a specially bound Symposium Volume published by Messrs. Butterworths (London).

P. BIELY

XVI INTERNATIONAL CONFERENCE ON COORDINATION CHEMISTRY

Dublin, 19-21 August 1974

Scientists from 37 countries attended. Amongst them were representatives from all five continents, including some of the developing countries. Rather large delegations were present from Canada, Denmark, Federal Republic of Germany, France, Ireland, Italy, Netherlands, Switzerland, UK, USA, and USSR. The total attendance, including accompanying members, was about 650.

The programme was divided into five sections in each of which a plenary lecture, several session lectures, and a large number of contributed papers,

were read. The five plenary lectures will be published in *Pure and Applied Chemistry* (scheduled Vol. 44, No. 1, 1975). Abstracts of other papers read at the Conference, together with papers accepted on reserve, are published in the *Proceedings of the XVI ICCG*, copies of which may be obtained by purchase from the Organizers (Department of Chemistry, Trinity College, University of Dublin, Dublin 2, Ireland).

Section I. Biological Aspects of Coordination Chemistry

In his plenary lecture entitled 'Functional and Conformational Properties of Metalloenzymes', B. L. VALLEE (Harvard University) discussed how chemical, spectral, and kinetic data on carboxypeptidase A in solution and in the crystal state compared with the results of X-ray structural analysis of the enzyme crystals. He concluded that the physical state of an enzyme was a significant experimental variable that likely induced changes in function-related-conformation. Because the kinetic properties of carboxypeptidase crystals differed markedly from those of solutions, enzyme-substrate model building, based on kinetics in solution, would seem of questionable value in solving mechanistic problems.

Four session lectures were given in this Section. G. N. SCHRAUZER (University of California, San Diego) talked about cobalt-carbon bond cleavage reactions in corrins and vitamin B₁₂ model compounds. G. L. EICHHORN (Baltimore Hospital) described the influence of bivalent metal ions on genetic regulation. R. D. GILLARD (University College, Cardiff) talked about bacteria and metal complexes. In a lecture describing the relevance of coordination chemistry to medicine, B. SARKAR (University of Toronto) presented in quite a dramatic way how molecular design in coordination chemistry might bring new approaches in the treatment of metal related diseases.

Thirty-six contributed papers were also read in the Biological Section, which excited sufficient interest to ensure that this area of study was likely to be a well supported one at future coordination Conferences.

Section II. Physical Methods and Bonding

Because of the large number of papers accepted in this Section, two parallel sessions were run concurrently.

In his plenary lecture 'On the Information Content in a Weakly Structured Absorption Band', C. J. BALLHAUSEN (University of Copenhagen) struck a critical note, when he stated that 'all parameters derived from weakly structured bands are to be viewed with caution'. After developing a theoretical description of how broad structureless bands in medium-size molecules of inorganic complexes arose from the crowding together of vibrational levels (each 1-100 cm⁻¹ broad), the dangers of assigning unresolved structural bands observed well above absolute zero to (a) lower symmetry, (b) spin-orbit coupling, (c) Jahn-Teller effects, and (d) 'antiresonances', were elaborated. Session lecturers included B. R. MCGARVEY (University of Windsor), who reported on single crystal ESR of d¹ and strong field d⁵ complexes. S. F. A. KETTLE (University of East Anglia) discussed the vibrational spectroscopy of solids, taking into account anharmonic, multipolar coupling, molecular orientation, and nonzone centre effects. J. A. IBERS (Northwestern University) described recent structural studies of transition metal complexes, including nitrosyl compounds. The technique of matrix isolation (in solid argon at 20 K) as applied to coordination compounds was described by J. J. TURNER (University of Newcastle), with particular reference to (a) spectral

studies of individual molecules which normally would show association or reactivity, (b) coordination of metal atoms with a reactive substrate to generate species unstable above 50 K, (c) 'molecules' of low-coordination number, (d) study of carbonyl intermediates formed by flash photolysis.

In addition, 84 contributed papers were read.

Section III. Inorganic Reaction Mechanisms

Forty-seven contributed papers relating to kinetics and mechanism were given in this Section. The plenary lecture 'Intra-Molecular Electron Transfer' presented by H. TAUBE (Stanford University), dealt with attempts to measure the rates of electron transfer in precursor complexes in which metal atoms were bridged and which led to a net redox process. A discussion of traditional oxidation-reduction reactions was followed by one on a special class of reactions in which a ligand attached to an oxidizing centre was converted to a reducing agent *in situ* and, in turn, reduced the oxidizing metal centre. Mixed valence complexes were also treated. L. CATTALINI (University of Venice) spoke on the role of chelating ligands in substitutions at planar, tetra-coordinated d^8 complexes, A. MCAULEY (University of Glasgow) on redox reactions between metal ions and sulfur-containing ligands, M. D. JOHNSON (University College, London) on oxidatively-induced reactions of organo-metallic complexes, H. DIEBLER (Max-Planck Institut, Göttingen) on substitutions of octahedral metal complexes, and J. E. BALDWIN (MIT) comprehensively reviewed the factors involved in the reversible binding of O_2 to iron(II) macrocyclic complexes.

Section IV. Reactions of Coordinated Ligands including Catalysis

J. LEWIS (University of Cambridge) gave a plenary lecture entitled 'Reactions of Olefins with Some Group VIII Metal Carbonyls'. He reviewed the basic structural forms of polynuclear carbonyls and described the way in which ^{13}C NMR spectroscopy was used to determine the mechanism of fluxional interchange within these aggregates. The variety of pathways for exchange of carbonyl groups was established and correlated with the structure of the polynuclear species. The facile amphoteric electronic behaviour of duodecacarbonyls of iron, ruthenium, and osmium, was related to their orbital structures. The discussion emphasized three aspects of the chemistry: (1) the nature of the bonding and the fluxionality exhibited by polynuclear carbonyls of Group VIII, (2) the variation in the reactivity of the trinuclear clusters to inorganic donors, (3) the structure and reactivity of simple unsaturated organic groups with the polynuclear carbonyls. Much of the chemistry of these polynuclear aggregates differed very significantly from that of the simple metal systems. Such systems, in which organic groups were bonded to a cluster of metal atoms, might provide potential analogues for study of the structure and reactivity of organic species on metal surfaces or with heterogeneous catalytic systems.

The olefin complexes of zerovalent nickel were the subject of C. A. TOLMAN's (E. I. du Pont de Nemours, Wilmington) Session lecture, while P. HEIMBACH (Max-Planck Institut, Mülheim) discussed metal-catalysed cooligomerizations. The influence of electronic and steric effects on the reactivities of ligated species was described for metal coordinated aminoacids by R. UGO (Institute of Inorganic Chemistry, Milan) and for complexes with bulky tertiary phosphine or arsine ligands by B. L. SHAW (University of Leeds). In addition there were 44 contributed papers.

Section V. Coordination Chemistry and the Environment

The plenary lecture entitled 'The Influence of Natural and Synthetic Ligands on the Transport and Function of Metal Ions in the Environment' was given by A. E. MARTELL (Texas A. and M. University). The nature of the toxic metals, mercury, lead, and cadmium, as they existed in the environment and their transport through various parts of the ecosystem were examined. The constitution and properties of naturally occurring ligands as well as of those ligands now in largescale commercial production were considered. An analysis of the current controversy over the substitution of nitrilotriacetic acid (NTA) for tripolyphosphate in detergents, indicating that NTA should be favoured for largescale application as its environmental impact, appeared to be minimal. J. M. WOOD (University of Minnesota) described metabolic cycles for toxic elements in the environment. D. F. MARTIN (University of South Florida) discussed the application of coordination chemistry to some contemporary problems in biology, including the 'red tide'. E. HÖGFELDT (KTH, Stockholm) described geochemical problems. H. A. C. MCKAY (AERE, Harwell) spoke on the role played by the coordination chemistry of ruthenium, especially that of nitrosyl-Ru(III) in the reprocessing of spent nuclear fuel. Five contributed papers were read in this Section and there was a useful general discussion on environmental chemistry in which both academic and industrial chemists took part.

The meeting was held jointly at Trinity College and University College, Dublin. A varied and extensive social programme included receptions at the two Universities, a State reception at Dublin Castle, and a visit to the famous Abbey Theatre (sponsored by the Irish Tourist Board).

D. A. BROWN
W. J. DAVIS

XIV PRAGUE MICROSYMPOSIUM ON MACROMOLECULES: CROSSLINKING AND NETWORKS

Prague, 26-29 August 1974

There were 224 active participants (144 from abroad) at this meeting. Seven of the eight announced lectures were presented (that of Prof. N. S. ENIKOLOPOV was cancelled); full texts will be published in *Pure and Applied Chemistry* in 1975 (scheduled Vol. 43, Nos. 1-2) and by Butterworths as a separate volume. Of the total number of 70 short communications presented during the Microsymposium, some 30 will appear in the *Journal of Polymer Science, Part C (Polymer Symposia)*.

Problems of crosslinking statistics and network topology were discussed in detail and supplemented by a number of interesting results on systems important in practice. Attention was also paid to the formation of inhomogeneities and methods of their characterization, to the theoretical and experimental description of elastic and rheoptie behaviour of networks, and their interaction with diluents.

Prof. M. GORDON discussed current problems of crosslinking statistics based on the theory of cascade processes with particular emphasis on the transition from macroscopic to small systems, cyclization, and experimental evaluation of systems near to the gel point. Prof. T. E. LIPATOVA dealt with special features of network formation affected by strong intermolecular interactions. Formation of polyurethane networks and anionic polymeriza-

tion of oligoester acrylates was explained in detail as a relevant example.

Prof. M. SHEN analyzed in detail the thermoelastic equilibrium behaviour of networks and reviewed experimental methods and calculation procedures for the energetic component of the retractive force. Prof. R. H. WILEY reviewed the copolymerization behaviour of divinylbenzene isomers with styrene and discussed the differences in the structure and properties of the products.

Prof. P. REMPP explained new ways of preparing polymer gels by end-linking of living precursor chains and analyzed the equilibrium elastic and sorption behaviour of gels in the light of current theories of network elasticity. Prof. B. E. EICHINGER brought forward a new theoretical treatment of network elasticity, based on the network topology and allowing for conformational restrictions due to crosslinks. Prof. G. REHAGE made an analysis of a complex experimental study of chemically and physically crosslinked systems, with particular reference to systems where both types of crosslinks occurred simultaneously. Formation of ordered regions and stereocomplexes was also discussed.

The establishment of a close connection between network formation, which determined the network topology, and properties might be regarded as one of the most important contributions of the Microsymposium. These ties were demonstrated by a great number of communicated results; several theoretical approaches to the problem were also presented. It became apparent that the theoretical approach could contribute importantly to the control of crosslinking processes and elucidation of the crosslinking mechanism.

B. SEDLÁČEK

IV INTERNATIONAL CONFERENCE ON RAMAN SPECTROSCOPY

Brunswick, Maine, 25-29 August 1974

This meeting was held on the attractive campus of Bowdoin College. E. R. LIPPINCOTT was Chairman of the Organizing Committee, J. E. GRIFFITHS was the hard-working Secretary, J. R. DURIG was Programme Chairman, and D. W. MAYO did an excellent job with the local arrangements. The Optical Society of America, the National Science Foundation, and IUPAC were sponsoring organizations.

These Conferences have shown a steady growth in size, reflecting the rapid growth of interest in Raman spectroscopy. Nevertheless, the Organizing Committee was taken aback by the number of attendees and the number of papers. Both came close to taxing the facilities available. There were approximately 410 scientists and 80 nonscientists present, and 284 papers were scheduled. A serious effort was made to encourage graduate students and young scientists to attend by the provision of reduced rates and special grants.

The papers were divided into three categories: 50-minute invited ones, 25-minute invited ones, and 15-minute contributed ones. There were 44 in the first two categories, and 240 contributed papers. Mornings were devoted to single sessions containing from two to six plenary lectures. In the afternoons there were four simultaneous sessions. The attendees had a wide international distribution; at least a dozen countries from outside North America were represented on the programme. The largest contingent of foreign papers was from France (36), followed by Federal Republic of Germany (22), UK (14), and Italy and Japan (9 each).

The programme constituted a very good representation of current work in Raman spectroscopy. Sessions were devoted to Instrumentation and New Techniques; Molecular Structures; Nonlinear, Resonance, and Electronic Raman Spectroscopy; Solid-state Studies; Band Shapes; Biological Applications; and Polymers. Among the invited speakers were I. R. BEATTIE, J. R. DURIG, T. HIRSHFELD, M.-L. JOSIEN, J. L. KOENIG, E. D. SCHMID, J. F. SCOTT, T. G. SPRIO, B. P. STOICHEFF, and G. R. WILKINSON. Nearly 70 papers dealt with the solid state, and about 44 papers had the phrase 'resonance Raman' in the title. Some interesting experimental developments were described, especially by M. DELHAYE and coworkers, by A. B. HARVEY, and by T. HIRSHFELD.

There was a small, but interesting and useful instrument exhibit. The meeting afforded good opportunities to meet and talk with others, because most of the attendees stayed on campus and ate in the same dining hall. A coffee break in midafternoon provided another occasion to mix informally.

The main fault the writer found was that the programme was too full and the pace too fast. Papers were scheduled to start from 8.30 to 17.30 for four consecutive days, and to 15.15 on the fifth. In hindsight it would have been better to have used an extra day, and to have had a free afternoon in the middle of the meeting. (Many of the attendees complained that they had no opportunity to see the beautiful Maine coast on which Brunswick is located.) In addition there was some problem getting to papers in different sessions, because the meeting rooms were in separate buildings and the sessions were not always kept on schedule. On the whole, though, the Conference was very well organized and run, the programme was excellent, and the site was a good one. Because the writer was a member of the Organizing Committee he hesitates to congratulate that group, but he was pleased with its work.

The proceedings of the Conference will not be published. The next Conference will be held in Germany in 1976 under the chairmanship of Prof. E. D. SCHMID (Freiburg i. Br.).

F. A. MILLER

I IUPAC CONFERENCE ON ORGANIC SYNTHESIS **Louvain-la-Neuve, 26-30 August 1974**

Three hundred and fifty chemists from 28 nations took part in this first Conference on Organic Synthesis, of which 33 are affiliated to IUPAC. It was organized by the three units of the Department of Chemistry of the University of Louvain, namely, Laboratory of General and Organic Chemistry (GEOR unit, under Prof. A. BRUYLANTS), Laboratory of Organic Chemistry of Synthesis (ORSY unit, under Prof. L. GHOSEZ), and Laboratory of Organic Chemistry (ORGA unit, under Prof. H. G. VIEHE).

The opening of the academic session took place at 9.30 on 26 August in the STUDIO auditorium (Avenue Georges Lemaitre). Colonel BEM SEGERS was present on this occasion, representing His Highness King Baudouin, who accepted to patronise the Conference. Prof. VANDER VORST, Vice-President of the Academic Council of the Catholic University of Louvain, welcomed the participants in the name of Mgr. MASSAUX, Rector of the University, and presented the transferred University into its new status.

Prof. P. YATES (University of Toronto), the Secretary to the IUPAC Division of Organic Chemistry, evoked the role of the International Union of Pure and Applied Chemistry. He reminded participants that the Division of

Organic Chemistry, among other activities, had already patronised two series of biennial meetings: the Symposia on Natural Product Chemistry and the Conferences on Physical Organic Chemistry. This had brought to light the necessity to start a series of scientific meetings aimed at Organic Synthesis. In his speech, Prof. BRUYLANTS, President of the Organizing Committee, stressed the importance of organic chemistry as the main factor of the economic development and democratization of a country. In its constant progress today, it controlled, more than ever, the habitat of man, his clothing, his nourishment, his health. For the last few years, its industrial applications had become famous and we were happy and proud of its outcome.

The workshops followed next. They were centred on the fundamental problems of organic synthesis: new general methods, physical activation, surround effect, stereochemical control, and industrial organic synthesis. Fourteen plenary lectures (to be published in *Pure and Applied Chemistry* during 1975, scheduled Vol. 43, Nos. 3-4) were consecrated to these different themes and the participants took part in their discussion:

Cyclopropanation of Silyl Enol Ethers: A Powerful Synthetic Tool—J. M. CONIA (France)

Chiral Recognition in Complexation of Guests by Designed Host Molecules—D. J. CRAM (USA)

Importance of Conformation of the Tetrahedral Intermediate in Hydrolysis of Esters and Amides—P. DESLONGCHAMPS (Canada)

Effect of Pressure on Electronic States of Organic Solids—H. G. DRICKAMER (USA)

Asymmetric Catalysis by Chiral Rhodium Complexes in Hydrogenation and Hydrosilylation Reactions—H. B. KAGAN (France)

Synthetic Studies in the Field of Natural Products—Y. KISHI (Japan)

Two-phase Reactions in Chemistry of Carbanions and Halocarbenes.

A Useful Tool in Organic Synthesis—M. MAKOSZA (Poland)

Applications of Thallium(III) Nitrate (TTN) to Organic Synthesis—A. MCKILLOP (UK)

Singlet Oxygen: A Reagent in Organic Synthesis—G. OHLOFF (Switzerland)

Use of Polymeric Reagents in Organic Synthesis—A. PATCHORNIK and M. A. KRAUS (Israel)

Industrial Synthesis of Terpene Compounds—H. POMMER (Germany)

Use of Kinetically Generated Unstable Enolate Ions in Regiospecific Formation of Carbon-Carbon Bonds: Specific Applications to Annulation Processes—G. STORK (USA)

Novel Approaches to Alkylations—B. M. TROST (USA)

Total Synthesis of Vitamin B₁₂—R. B. WOODWARD (USA)

Two seminar sessions took place on the Wednesday and Thursday afternoons. They included 17 communications, also followed by discussions. The choice of the themes and of the plenary lecturers was made by a Committee composed of international scientists. This Committee had at its disposition the result of a large enquiry made by the Organizers during the first half of 1973, among 100 specialists who had accepted to answer questions in pointing out which were the latest problems in organic synthesis. This procedure enabled presentation of a scientific programme particularly well adapted to the precise needs of the present. A large number of the participants took part in the working sessions and the discussions were really lively and fruitful.

A. BRUYLANTS

IV POLISH CONFERENCE ON ANALYTICAL CHEMISTRY

Warsaw, 26-31 August 1974

Six years after the III Polish Conference on Analytical Chemistry in 1968, the Analytical Chemistry Commission of the Polish Academy of Sciences organized the IV Conference, as previously in cooperation with the Polish Chemical Society and under the auspices of IUPAC. This Conference was held at the University of Warsaw, where in the beautiful stylish XVI-century palace was located the Conference office. All lectures took place in the nearby located auditorium.

In spite of the official name of the Conference, the 130 (of the total 600) participants from abroad contributed significantly to its international flavour. Countries that were represented were Belgium, Bulgaria, Czechoslovakia, Egypt, Federal Republic of Germany, France, German Democratic Republic, Hungary, Iran, Italy, Japan, Netherlands, Romania, Sweden, Switzerland, UK, USA, USSR, and Yugoslavia.

At the Opening Ceremony in the Auditorium Maximum, the President of the Analytical Chemistry Commission of the Polish Academy of Sciences, Prof. W. KEMULA welcomed the participants as the Chairman of the Organizing Committee. Among the other addresses given should be mentioned specially those of the President of the Polish Academy of Sciences, Prof. W. TRZEBIATOWSKI, and of the President of the Analytical Chemistry Division of IUPAC Prof. N. TANAKA. The first of the plenary lectures* was given by Prof. J. MINCZEWSKI (Poland), who summarized the thirty years of development and present status of analytical chemistry in Poland.

The plenary lecture of Prof. N. TANAKA (Japan) was devoted to the mechanism and characteristics of electrode reactions of analytical interest. The author showed the importance of studies of such processes especially in trace analysis and for establishing the universal potential scale in different solvents. It was shown that careful examination of systematically classified electrode reactions may lead to the best use of them as well as of electro-analytical techniques for determination of substances.

On electroanalytical problems spoke also Prof. E. PUNGOR (Hungary), who considered in detail voltammetry on silicone rubber based graphite electrodes. The numerous examples presented by the speaker indicated the possibility of employing sensors for the anodic polarization range, being of significant value in pharmaceutical analysis and for measurements carried out *in vivo*. Special regard was paid to flow systems in which modern analytical applications were of increasing interest.

Another electrochemical topic was treated in detail by Prof. W. SIMON (Switzerland), who clearly indicated the scientific way which led him from model calculations to the design and synthesis of neutral carriers employed in liquid-state ion-selective electrodes. This logical treatment was rewarded by obtaining, as a final product of investigation, electrodes which, when used as chemical sensing elements, exhibited strictly defined properties and selectivities. The recent results presented, indicated that this new field develops continuously.

Prof. J. ZYKA (Czechoslovakia) had a difficult task in his lecture, in defending titrimetric methods against the constant attack of instrumentation in analytical chemistry. However, he was able to convince his audience that new

*Scheduled for publication in *Pure and Applied Chemistry*, Vol. 44, No. 3 (1975)

titrimetric methods were being developed and their importance was still high not only in direct determinations, but also in the study of mechanisms and rates of chemical reaction, *etc.*

The first of the lectures dealing with organic analysis was that of Prof. F. PELLERIN (France), who spoke on new trends in organic functional analysis, which presently aimed at analytical determinations as well as structural studies. The speaker pointed out that only the application of instrumental methods, being complementary to classical ones, gave satisfactory results. In his presentation Prof. PELLERIN showed many examples of such procedures, based on potentiometry, polarography, together with a broad range of spectroscopic techniques.

To problems of organic microanalysis was devoted the lecture of Prof. N. E. GEL'MAN (USSR). The speaker discussed the mechanism of reactions occurring in the course of destructive oxidation of organometallic compounds, indicating the possibility of obtaining different final products. The reaction mechanism, as was shown, may be changed in the required direction by addition of some substances and due to temperature variations. In this lecture a suggestion was made that application of such instrumental methods as X-ray fluorescence was especially useful for the rapid and sufficiently precise determination of heteroatoms.

Two lectures were devoted especially to environmental analysis. The first one, read from the manuscript in the absence of the author, Prof. K. H. MANCY (USA), discussed the general aspects of analytical chemistry in water pollution control, considering in more detail the design of the measurement systems. The next lecture, by Prof. A. LIBERTI (Italy), summarized recent results in air pollution monitoring. In giving a general classification of methods used currently in air pollution control, he paid special attention to the determination of carbon monoxide, sulfur dioxide, nitrogen oxides, and oxidants, indicating the possibilities of analysis of the sample, remote sensing or long path measurements on site.

The presentation of Prof. YU. A. ZOLOTOV (USSR) summarized methods of determination of trace elements currently used in the USSR Geological Survey. The role of preconcentration was emphasized particularly and the most important reagents used in different procedures were indicated. As an example of analysis of unusual objects, the analysis of lunar samples was considered in some detail.

A completely different object of analytical investigation was treated by Prof. J. LENIHAN (UK). Activation analysis in clinical and biological research allowed the determination of trace impurities and minor constituents which played an extremely important role in proper functioning of the human body or were responsible for several diseases. The thorough study of those problems might lead to establishing relationships between chemical environment and living organisms. The development of activation techniques also enabled the direct study of an intact body and the investigation of dynamic metabolic processes. The speaker suggested that the limited success of activation analysis until now was attributable more to lack of imagination than to shortcomings in the technique.

Microanalytical techniques in the application to extreme trace analysis were discussed by Prof. G. TÖLG (FRG). Based on his rich experience, he posed the sound suggestion that only results obtained from a combination of several analytical techniques served as proof of the validity of direct instrumental methods and could eliminate errors arising, for example, from faulty standards. The use of micro and ultramicro techniques could help in

elimination of the sources of systematic errors. Various examples from the author's Institute, concerning the analytical characterization of pure metals and determination of traces in organic as well as inorganic matrices, supported those views.

The problems of trace analysis were also tackled by Prof. T. S. WEST (UK), who spoke on developments in atomic spectrometry. Progress in this area was continuous and improvements might be found in new atomization techniques and application of atomic fluorescence spectroscopy. The speaker indicated time-resolved nondispersive fluorescence as a method of great prospects in the near future.

The last two plenary lectures were devoted to some statistical approaches in analytical chemistry. The question of the methodical consequences of 3- σ criterion was discussed by Prof. K. DOERFFEL (GDR). He indicated that the significance principle might be taken as the basis for extending the limits and possibilities of analytical methods. Further chemical information about the system might help in improvement of detectability, selectivity, etc. This speaker pointed out that in analytical chemistry an increasing role was played by transient phenomena. Practical examples illustrating those principles were given mainly for spectroscopic methods.

Another approach was presented by Prof. C. LITEANU (Romania), who discussed the limit of detection. To define it he used a two-step model, based on a false detection probability to which corresponded a detection limit, as well as on a proper detection probability. To estimate the value of the limit two procedures were given.

The participants of the Conference presented 244 original communications in the following sections: general problems, organic analysis, trace analysis, environmental analytical chemistry, and analysis of inorganic products. In spite of shortage of time, some especially interesting discussions took place on topics concerning chromatographic theory and practice, application of electroanalytical methods, and atomic spectroscopy.

During the Conference several scientific excursions to analytical laboratories were organized, which enabled the participants to compare the everyday laboratory work with the papers presented at the Conference. The social events which were organized included a cocktail party in the Staszic Palace—the site of the Polish Academy of Sciences, and an opera performance.

A. HULANICKI

IV DISCUSSION CONFERENCE ON MACRO- MOLECULES: HETEROGENEITIES IN POLYMERS

Mariánské Lázně, 2-5 September 1974

There were 124 active participants (72 from abroad) in this IUPAC-sponsored meeting. Fifteen of the announced lectures were presented (those of Prof. CH. SADRON and Dr. G. P. GLADYSHEV did not take place): some of these papers would be published during 1975 in *Pure and Applied Chemistry* (scheduled Vol. 43, Nos. 1-2). The topics of this Discussion Conference were intentionally restricted mainly to the physical aspects of formation and properties of heterogeneities in various polymer systems. These problems belong to the highly topical ones, both from the scientific and practical standpoint.

Prof. H.-G. ELIAS devoted his lecture to the problems of polymolecularity and polydispersity which reflect the molecular heterogeneity of polymers.

The lecture not only helped to improve the systematics of findings obtained so far, but also elucidated some practical problems of investigation of associating systems. Prof. V. V. KORSHAK demonstrated the role of chemical defects in polymers with anomalous repeat units. A number of examples illustrated the effect of heterounits on the chemical and physical properties of polymers.

The lecture of Prof. J. E. HEARST was an introduction to the discussion of molecular heterogeneities in DNA. A study of simple sequences in *Drosophila melanogaster* DNA was reported. Prof. B. VOLLMERT explained his view of the problem of the mutual interpretation of polymer molecules, in connection with investigation of the structure of the noncrystalline polymer phase. He demonstrated by means of his experimental results that the degree of conversion approximately corresponded to the degree of interpenetration, and showed conditions which controlled the formation of interpenetrated structures and methods of investigation of their properties.

Prof. R. G. KIRSTE used light scattering, X-rays, and neutron scattering data to demonstrate that amorphous solid polymers behaved similarly to low molecular weight liquids. He also described two methods of investigation of conformational changes and particularly stressed the great prospects offered by the low angle neutron scattering method. Prof. R. HOSEMANN discussed the problem of supermolecular heterogeneities in terms of paracrystallinity; the crystalline phase was, in fact, a mixture of isolated micro-paracrystallites. Polyethylene was used as an example to show how an organized structure was formed in which knots formed just microparacrystallites; the stability and retransformation of the knots were studied.

Prof. A. PETERLIN studied diffusive transport in polymer solids with alternating crystalline-amorphous regions. Each anisotropy of morphology automatically led to anisotropy of diffusion. Conditions which influenced this relationship were described. Prof. K. C. FRISCH reported the results of an investigation of topologically interpenetrating polymer networks, based on a study of their mechanical and thermal properties in relation to their morphology. It appeared that the conditions of formation of such networks could be chosen so as to obtain systems with optimal properties.

Prof. M. KRYSZEWSKI investigated the effect of molecular and supermolecular heterogeneities on the charge transfer in polymers. The author analyzed in detail the effect of chemical and physical factors which influenced trapping phenomena in polymers. Prof. A. S. ARGON discussed in his lecture the role of natural and synthetic heterogeneities in the mechanical behaviour of glassy polymers. Heterogeneities led to a nonuniform energy distribution and propagation in polymers, which might explain a number of aspects of their mechanical properties.

Prof. L. E. NIELSEN investigated properties of a two-phase system consisting of an elastic material in a rigid matrix, especially in connection with the formation of fractures. He showed ways and means of how to follow the fracture process using two-phase systems. Prof. YU. S. LIPATOV in his lecture elucidated some aspects of the role of interface phenomena in the formation of micro- and macroheterogeneities in multicomponent systems. He discussed cases when the phase boundary was permeable or impermeable for the polymer and showed the relationship between microheterogeneities and macroheterogeneities. Finally, Prof. M. PEGORARO reviewed conditions affecting the formation and properties of some two-phase polymer systems and demonstrated his conclusions on several experimental examples.

Although the programme of the Conference was restricted to physical aspects of the given subject, the formation and properties of heterogeneities in polymers appeared to be a very involved and many sided problem. So far a vast amount of experimental material had been gathered, but one was still very far from an understanding of all the diverse phenomena included in the term of 'heterogeneity in polymers'. Much attention had also been devoted to the search for new methods which provided a deeper insight into this phenomenon or allowed it to be characterized using new physical parameters. The lectures and discussions held at the Conference outlined the existing state of knowledge in this field and indicated routes for further progress.

B. SEDLÁČEK

IV INTERNATIONAL SYMPOSIUM ON MEDICINAL CHEMISTRY

Noordwijkerhout, 9-13 September 1974

The Symposium was organized by the Medicinal Chemistry Division of the Royal Netherlands Chemical Society in cooperation with the Medicinal Chemistry Division of the Flemish Chemical Society, under the sponsorship of the IUPAC Section on Medicinal Chemistry, Fédération Internationale Pharmaceutique, Royal Netherlands Chemical Society, and Royal Netherlands Association for Advancement of Pharmacy. Its realization was made possible by financial aid and/or guarantees by the two last-mentioned sponsors and a large number of companies active in the pharmaceutical-chemical field. In the preparatory period the Organizing Committee was shocked by the sudden death at the early age of 44 of Prof. H. CORRODI, who had accepted an invitation for a plenary lecture. He was a great scientist and a marvellous man who will be missed in both capacities.

Held at the Congress Centre 'Leeuwenhorst' at Noordwijkerhout, the Symposium was attended by 350 active and 68 accompanying participants from 25 countries.

Sixteen main lectures, 10 thirty-minute lectures, and 32 short communications were devoted to the following topics and features.

- Inflammation: A Biological and Chemical Outlook; plenary opening lecture by DORT
- Medicinal Chemistry related to Central Transmitters (5 main lectures by ANDÉN, GRAHAME-SMITH, KOBINGER, SANDLER, and STÄHLE, 2 thirty-minute lectures, and 14 short communications)
- Microsymposium: Medicinal Chemistry of 1,3-Indandiones (2 main lectures by DUBURS and DURDEN, 1 thirty-minute lecture, and 3 short communications)
- Medicinal Chemistry of Thrombolytics and Antithrombotic Agents (3 main lectures by BRAKMAN, MILLS, and THOMAS, 4 thirty-minute lectures, and 4 short communications)
- Chemotherapy of Parasitic Infections; Antiprotozoal Agents and Anthelmintics (2 main lectures by ELSLAGER and LOEWE, 1 thirty-minute lecture, and 4 short communications)
- Chemical Structure and Pharmacokinetics: A Basis for the Modulation of Therapy and Toxic Action (3 main lectures by ARIËNS, BECKETT, and LIEN, 2 thirty-minute lectures, and 7 short communications)

—In the Closing Session the Concluding Remarks were made by ALBERT (Australia).

A large number of accompanying participants took part in the events of the ladies' programme. One of the highlights of the social programme was the reception on behalf of the Government of the Netherlands by officials of the Department of Public Health and Environmental Control and the Department of Science and Education in the wonderful new Van Gogh Museum in Amsterdam.

From the concluding remarks by Prof. ALBERT we cite the following sentences:

'I am glad of this opportunity to make some concluding remarks: they will be few because I am sure that your ears are ready to enjoy some rest after the feast of good things that we have been hearing.

'However, I hope that you can participate with me in a short consideration of what the composition should be of an ideal Symposium on Medicinal Chemistry. The great difficulty, you may agree, is in getting the right proportion of "medicinal" to "chemistry". If the biology predominates, as it did in Milan, too little expression can be given to the *noun* in our title, while the *adjective* runs wild. Yet we must be equally careful not to make the programme largely chemical, for then we would not be obviously different from those many chemical symposia, on selected topics, which seem to be taking place all the time and in almost all countries.

'The delightful feature of the present Symposium was that it held a good balance between these extremes, so that the reported discovery of new compounds (sometimes described down to the last detail of the reagents used) led on, in a very natural way, to biological testing in the laboratory, and often from there into the clinic from which points the reported results seemed to lead back to fresh, and even more relevant chemistry.'

As was expressed by a large number of participants, the fact that accommodation and lectures were in the Congress Centre ensured excellent possibilities for personal contacts and discussions. We would certainly recommend that in the organization of future symposia in this series this point be taken into consideration.

Undoubtedly, the pleasant accommodation of the Congress Centre 'Leeuwenhorst' and the considerate and good care of its staff contributed to the pleasant remembrance of the Noordwijkerhout Symposium.

The full text of the main lectures was published by Elsevier Scientific Publishing Co. at the end of 1974. A limited number of booklets containing Abstracts of all lectures and communications (80 pages) is still available and can be ordered by remitting Dfl. 5 (Holland) or Dfl. 7.50 (other countries) to account nr. 47.81.76.104 (Chemie Congressen V) at the AMRO Bank, Oss (Netherlands).

J. MAAS
W. TH. NAUTA

II INTERNATIONAL SYMPOSIUM ON INORGANIC PHOSPHORUS COMPOUNDS

Prague, 9-13 September 1974

The Symposium took place in the Grand Hotel International in Prague, sponsored by IUPAC, and organized in collaboration with the Czechoslovak Committee for Chemistry, the Czechoslovak Chemical Society, the Prague

Institute of Chemical Technology, and the Pedagogical Faculty in Ústí nad Labem. It followed the tradition of the 1st Symposium (Prague, 1970), which was to establish a forum for an international exchange of views and for discussions between chemists working in the field of inorganic phosphorus compounds in the widest sense, every 3 or 4 years.

About 300 participants took part in the II Symposium. It had an international character. There were 49 scientists from the host country; the rest came from 19 countries of North America, Asia, and Europe. To enable younger experts to take part in the meeting, the Organizers granted a 60% reduction of the registration fee to 10% of the participants. The Symposium in Prague was followed by the V International Conference of Organic Phosphorus Chemistry in Gdańsk (16-21 September 1974).

The programme was divided into ten thematic groups; there were 16 plenary lectures* and 110 contributed lectures. Though a great number of contributed lectures were expected to take place in two thematic groups, the Organizers intentionally arranged for the relatively large number of 16 plenary lectures to be given in order to create intensive contacts between all the participants during the whole course of the Symposium.

The Symposium had the character of a workshop. In his opening speech, Dr. W. WANĚK welcomed the participants. Then followed the welcoming speech by the Honorary Chairman of the Czechoslovak Chemical Society on behalf of the Organizers, Prof. F. ČUTA; the President of the Inorganic Division of IUPAC, Prof. V. GUTMANN; and Prof. A. A. VLČEK on behalf of the Czechoslovak Academy of Sciences. The Organizers deliberately abstained from any other official actions.

In Thematic Group I, devoted to Elementary Phosphorus and Lower Valency Compounds of Phosphorus, I. V. KIRSANOV (Kiev) presented the introductory lecture on the intensively developing chemistry of phosphorus iodides. He discussed the preparation and reactivity of PI_3 and P_2I_4 and their substitution reactions. He described minutely the interactions between P_2I_4 with red phosphorus and alkyl iodides, which leads to the formation of alkylated products such as hexaalkyliodophosphorane phosphonium penta-iodides $[\text{R}_3\text{P}(\text{I})-\text{PR}_3]^+\text{I}_5^-$ or hexaalkylbisphosphonium bistriiodides $(\text{R}_3\text{P}-\text{PR}_3)^{2+}2\text{I}_3^-$. These compounds were suitable as starting materials in the synthesis of tertiary phosphine oxides, trialkylphosphine sulfides, trialkylphosphines, and quarternary phosphonium salts. In this same Thematic Group, D. HEINZ (Berlin) presented a most interesting lecture on the chemistry of P_4O_6 , which mainly demonstrated that the foundations for the industrial production of the material had been laid.

In Thematic Group II, which concerned itself with Monomeric and Polymeric Phosphates and their Derivatives E. J. GRIFFITH (St. Louis) spoke on the chemical and physical properties of condensed phosphates. Besides a broad survey of the current state of this field of phosphorus chemistry, there were also discussed phase transitions of condensed phosphates, namely of $\text{Na}_4\text{P}_4\text{O}_{12}\cdot 4\text{H}_2\text{O}$ and $\text{Na}_3\text{P}_3\text{O}_{10}\cdot 6\text{H}_2\text{O}$ (in the presence of urea). The synthesis and properties of simple and complex polymetaphosphate glasses of alkali metals were the subject of a plenary lecture by R. C. MEHROTRA (Jaipur), which was read in shortened version by E. FLUCK (Stuttgart), because the author was prevented from attending the Symposium because of illness.

*Scheduled for publication in *Pure and Applied Chemistry*, Vol. 44, No. 3 (1975)

In Thematic Group III, which dealt with Phosphorus-Nitrogen-Compounds, H. A. LEHMANN (Dresden) spoke about results and problems in the formation of P-N bonds. On the basis of data gained from the literature and from his own experience, especially in the field of nucleophilic substitutions of chlorine by amines in P-Cl bonds, in the synthesis of phosphoric triamide under various conditions, considering the formation of P-N bonds by ammonolysis of P-O-P bridges in aqueous medium and by thermal condensation reactions, as well as by the condensing of NH_2 and OH ending groups of catenaphosphates in which the nitrogen was kept in the formation of P-NH-P bridges, the author evolved a series of principles to which very little attention had so far been paid, although these condensation and polymerization reactions had currently been carried out.

Thematic Group IV was devoted to Phosphorus in Ligands of Coordination Compounds. K. ISSLEIB (Halle) read a very exhaustive paper on aspects of the coordination chemistry of tervalent phosphorus. After introductory considerations of the various uses of coordination complexes containing tervalent phosphorus ligands and a discussion of the metal-phosphorus bond, the complex-forming behaviour of the derivatives of various structures in the reaction with metal salts was considered.

This review was completed by the lecture from M. I. KABATCHNIK (Moscow), read by T. YA. MEDVED on phosphoorganic complexones. It was demonstrated that the advance of synthetic methods had resulted in the development of a series of new and highly effective organophosphorus complexones operating over a broad range of pH values and exhibiting high selectivity. The principal method of producing these substances—polyaminopolyphosphoric acids—was condensation of carbonylic compounds with di- and polyamines and tervalent phosphorus compounds liable to diad tautomerism.

In Thematic Group V, Organoderivatives of Inorganic Phosphorus Compounds, R. VILCEANU (Timisoara) presented a comprehensive lecture on the chemistry of phosphorus acid amides. His lecture dealt mainly with the general preparative methods of phosphoric acid triamides, the fundamentals of the reactivity of phosphorus acid amides starting from the characteristics of the P-N bond, and some aspects of the applicative significance of these compounds.

H. W. ROESKY (Frankfurt/Main) opened the lectures in Thematic Group VI (Halides and Chalkogenides of Phosphorus) with a paper on the formation and reactions of sulfur-containing halogenophosphazenes. In this exceedingly interesting lecture the author dealt mainly with solvolysis reactions of these compounds with alcohols and different acids. He described different rearrangement reactions, where *S*-alkyl or *N*-alkyl compounds were formed.

In Thematic Group VII—Chemical Bond and Molecular Structure of Inorganic Phosphorus Compounds—R. A. SHAW (London) read an excellent lecture on aspects of structure and bonding in inorganic phosphorus compounds. Apart from the aspects of the structure and stability of cyclic phosphinoborines and acyclic N-P compounds, the lecture was devoted mainly to cyclophosphazenes. Ring shapes, conformations of substituents, bondlengths and angles, basicities, and other properties were discussed in some detail. The differences in ground state and perturbed state properties were also considered, and a comparison was made of the structural changes accompanying protonation of two phosphazenes, where X-ray crystallographic data were available for the three bases and their conjugate acids.

Finally, the current stage of theoretical concepts of bonding in these compounds was briefly surveyed.

H. BOCK (Frankfurt/Main) presented in his lecture on photoelectron spectra and bonding in phosphorous compounds, his remarkable conclusions resulting from the interpretation of the results of (low energy) photoelectron spectroscopy, which rendered possible a better appreciation of bonding in molecules. The author demonstrated that all valence electron ionization potentials of chemical species could be measured and could be generally interpreted making use of Koopmans' Theorem $IE_n = -\epsilon_{\text{J}}^{\text{SCP}}$, which provided a fruitful symbiosis between PE data and MO models. With the examples of elementary phosphorus (P_4), phosphine (PH_3), and their derivatives, phosphorus substituent effects in organic compounds and phosphorus multiple bonding, BOCK expounded his remarkable conclusion, which, among things, led him to the opinion that, for instance, bonding in P_4 was mainly due to the omnidirectional $3s$ orbitals, that lone pairs were more represented by $3p$ contributions, and that no $3d$ orbitals were needed at all to describe the electron distribution within the fascinating tetrahedron.

In Thematic Group VIII (Spectroscopic Methods in Phosphorus Chemistry), E. FLUCK (Stuttgart) presented a paper on X-ray photoelectron spectroscopy (ESCA) and its application in phosphorus chemistry. After discussion of this comparatively new method, he demonstrated how it could be applied to a great number of phosphorus compounds, and presented a number of facts about the binding energy data and the necessary corrections of Pauling's electronegativity values.

As a result of his long-standing work in this field, J. GOUBEAU (Stuttgart) presented a paper on vibration spectra and force constants of phosphorus compounds. This lecture gave an excellent survey of the findings in the field and demonstrated when, and to what extent, this already classical method could be applied either independently or in combination with other spectroscopic methods, especially with NMR spectroscopy, for the interpretation of spectra and the construction of such spectra from unknown phosphorus compounds.

In Thematic Group IX—Chromatography of Phosphorus Compounds—S. OHASHI (Fukuoka) presented a paper on the chromatography of phosphorus oxoacids. He discussed the chromatographic techniques, the separation mechanism and the characteristics of paper and thin-layer chromatography, paper electrophoresis, ion-exchange chromatography, and gel chromatography. He reported, as examples of the application of ion-exchange and gel chromatography, studies on the hot atom chemistry of ^{32}P in solid inorganic phosphates and those on the substitution reactions between diphosphonate (diphosphite) and polyphosphates.

Thematic Group X was devoted to New Applications of Inorganic Phosphorus Compounds. H. HARNISCH (Frankfurt/Main) surveyed the developments in the field of manufacture and use of inorganic phosphorus products. His lecture was concerned with basic products of industrial phosphorus chemistry and with their use in fertilizers, feed additives, and detergents. Special attention was paid to the present day development of the industry of phosphorus compounds, as well as to the different processes for manufacture and purification of wet process phosphoric acid, and by stimulation of the development of industrial phosphorus chemistry by the growing use of flame retardants.

In the last plenary lecture, W. WANĚK (Ústí nad Labem) called on the participants of the Symposium to concentrate their research work in the

field of inorganic phosphorus compounds more than ever on the immediate social problems, such as the problems of feeding mankind and the protection of life space. These problems called for speedy action to build up a perspective industrial production of fertilizers, where better use was made of phosphorus, and where water was protected from contamination by phosphates and nitrates. At the conclusion of his lecture he reported some work in the field of plant nutrition with covalent P-N compounds, especially amido-phosphazenes.

One aspect of the Symposium that received very favourable comment was the satisfactory balance between theoretical and practical phosphorus chemistry. The general calibre of the plenary lectures presented highly useful and broadly based surveys of phosphorus chemistry. The interaction between the spectroscopic and theoretical aspects of phosphorus chemistry was also demonstrated clearly. The increasingly important application of NMR to structure and bonding problems in phosphorus chemistry also received favourable comment. The introduction of carbon-13 NMR and the continued use of phosphorus-31 NMR were mentioned specifically. Preparative aspects of phosphorus chemistry also showed continuous progress.

The most persistent criticism was of the somewhat artificial subdivision of phosphorus chemistry into the inorganic and organic areas. The consensus view was that, with the exception of biophosphorus chemistry, all the various branches of phosphorus chemistry should be combined in future symposia. A further criticism that was voiced related to the fact that, despite its obvious industrial importance, there was no specific coverage of the chemical technology of phosphorus. The fact that very few papers stressed the reactivity of phosphorus compounds also received comment.

In considering possible improvements, the majority view was that in future the two existing series of inorganic and organic phosphorus symposia should be combined into a single set of meetings. In order to maintain the size of such symposia within reasonable limits it was suggested that future meetings be held approximately every 2 years. It was further suggested that future symposia be organized in terms of discrete topics, such as spectroscopy of phosphorus compounds, synthesis of phosphorus compounds, reactivity of phosphorus compounds, *etc.*

The Organizing Committee of the V Organic Phosphorus Chemistry Conference was to be contacted in Gdańsk, regarding a thorough discussion of any and all changes which were suggested in Prague. If the proposal for a combined phosphorus meeting did not come into effect, the III Inorganic Phosphorus Symposium would be held in 4 years. A brief discussion was held regarding a suitable location for such a symposium. Prof. ISSLEIB indicated his willingness to host it in Halle.

W. WANĚK

INTERNATIONAL SYMPOSIUM ON MACROMOLECULES

Madrid, 15-20 September 1974

This Symposium was held at the National Palace of Congress in Madrid, under the sponsorship of IUPAC, and was organized by the Instituto de Plásticos y Caucho of Madrid. It was attended by 995 people from 36 countries. The President of the Spanish Academy of Sciences, Prof. LORA TAMAYO, besides Prof. H. BENOÎT (President of IUPAC's Division of Macromolecules)

and Prof. J. FONTÁN (Chairman of the Symposium), presided over the Opening Session. Prof. FONTÁN welcomed the participants and spoke about the situation of macromolecular science in Spain as well as about the high level of scientific communications to be given during the Congress.

The scientific activities of the Symposium programme were:

- (i) 5 main lectures
- (ii) 28 invited lectures
- (iii) 370 scientific communications
- (iv) 3 reports from Working Parties of the IUPAC Macromolecular Division

The invited lectures and the scientific communications were divided into the following subjects:

1. New developments in polymerization
2. Chemical modifications and reactions on polymers
3. Properties in amorphous and crystalline polymers
4. Influence of structure on technical properties

The main lecturers were Profs. H. BENOÎT, P. J. FLORY, G. SMETS, J. FURUKAWA, and G. A. VINOGRADOV.

Prof. BENOÎT explained the theory and the application possibilities of the scattering of neutrons as a new technique to study configurations in polymers. The subject of structure, conformation, and morphology of polymers was developed by Prof. FLORY, whose well known theories were being supported by experimental results of some important research laboratories; the agreement of FLORY's theory with the results obtained by BENOÎT in determination of macromolecular dimensions in concentrated solutions and in the solid state (as explained by BENOÎT in his lecture) was to be noticed specially.

Prof. SMETS examined some photochemical reactions in relation to the physical properties of the solid polymeric matrix in which they were carried out. The three reactions considered by him were: photocrosslinking, photoisomerization, and photodissociation.

The mechanism of butadiene and of substituted diene polymerization using a catalyst composed of nickel carbonate, boron fluoride, and trialkylaluminium, was dealt with by Prof. FURUKAWA, who proposed for *cis*-polymerization a mechanism involving π -allylic polymer terminal with an intramolecular coordination of the double bond of the penultimate unit. He examined also the effect of additives to the catalyst. Electron-donor additives brought about the formation of *trans*-polymer. On the contrary, electron-acceptor additives gave *cis-trans* (1:1) polybutadiene.

Prof. VINOGRADOV developed the relaxation transition of linear polymers from fluid to rubbery state under the effect of deformation at temperatures above T_g . Predictions concerning the viscoelastic behaviour of polymers in uniaxial extension were possible on the basis of shear experiments under the conditions described by him.

The radical homo and copolymerization and related problems were the subject of several lectures. C. H. BAMFORD studied two kinds of photo-initiated system: (i) Group VII transition metal carbonyls in the presence of fluorolefins, and (ii) vanadium chelates and their derivatives. C. G. OVERBERGER in his lecture on catalysis by polymers, analyzed the hydrolysis of various nitrophenyl esters using poly-1-methyl-4-vinylimidazole and poly-1-methyl-5-vinylimidazole as hydrolysis catalysts. The catalytic action of these compounds was attributed to electrostatic and hydrophobic effects.

A. GUYOT reviewed the results obtained in his laboratory in the application of gas liquid chromatography to the study of radical copolymerization. This method had advantages, such as the possibility of following the individual consumption of each monomer and the fact that it allowed study of the copolymerization from the very start until high conversion. F. TÜDÖS presented a new improved method for determination of reactivity ratios as well as for estimation of the validity of the composition equation. The method was drawn from the hot radical theory, which was also explained by him. According to V. A. KABANOV's lecture, a chemical study of some apparently homogeneous systems was not quite satisfactory for a whole knowledge of their behaviour; some fundamental physical aspects were to be considered too. Among these aspects, he pointed out the action of complex forming agents and the microassociation of macromolecules.

In the ionic polymerization field the lectures given by D. C. PEPPER, M. SZWARC, and P. SIGWALT, were to be mentioned particularly. PEPPER gave a review of some results on cationic polymerization initiated by γ -rays, by carbocation salts, and by strong acids, especially HClO_4 , and concluded that the criteria for true living polymerization were not satisfied. On the basis of the fact that free ions and ion pair fractions depended, respectively, on the dielectric constant and on the solvating power of the solvent, SIGWALT explained the latest progress made in the field of reactivity of free ions and ion pairs in anionic polymerization. SZWARC defined the dynamic flexibility of molecular chains and its determination by studying the ESR spectra of radical anions formed by attaching two naphthyl end-groups to the investigated chains and reducing only one of them to a radical anion.

Six interesting lectures were devoted to the subject of chemical reactions on polymers. Those of D. BRAUN and R. C. SCHULZ dealt with chemical reactions as a useful help to investigate the properties of macromolecules. G. B. BUTLER studied a number of derivatives obtained from the 1:2 alternating copolymer of divinyl ether and maleic anhydride, some of which derivatives had been found to have antitumor effects.

A. CHAPIRO discussed graft copolymerization on acrylonitrile and its application to interpret the free radical peroxidation of most polymers. P. GIUSTI's lecture dealt with his recent results on both electroinitiated and electroinfluenced polymerization; he also proposed a classification of the electroinitiation processes and an algebraic treatment which agreed satisfactorily with the experimental results. J. GUILLET's lecture dealt with photochemical reactions in polymeric solids.

The lectures included in the third subject field were given by R. F. BOYER, R. HOSEMAN, A. PETERLIN, E. W. FISHER, A. KOVACS, P. KRATOCHVIL, and P. CORRADINI. Some of them (FISHER, CORRADINI) were devoted to chain conformations in relation with the order in various states of polymers. KRATOCHVIL reported the use of a light scattering technique to study multi-component polymer systems; this technique made it possible to determine the correct molecular weights of the components and parameters characterizing the thermodynamic interaction of unlike polymer molecules. BOYER and KOVACS developed some interesting aspects of thermal transitions in polymers. As for HOSEMAN and PETERLIN, their subjects were, respectively, the paracrystalline state of synthetic polymers and the environment induced crazing of crystalline polymers at cryogenic temperatures. HOSEMAN showed how a study of the paracrystalline state by means of X-ray analysis gave a lot of information on the molecular structure of polymers.

The lectures from the fourth subject area were given by S. LODGE, H. MARKOVITZ, A. M. NORTH, D. J. PLAZEK, J. HEIJBOER, J. F. JOHNSON, and M. KRYSZEWSKI. Rheology was treated by LODGE who pointed out the relation between rheological properties and molecular structure, and by MARKOVITZ who developed the theme of the superposition in rheology.

PLAZEK spoke of the viscoelastic behaviour of monodisperse polystyrene solutions in tricresyl phosphate, from the glassy to the terminal zones of response. KRYSZEWSKI and NORTH devoted their lectures to electrical properties of polymers. The former pointed out the two fields where new progress was being obtained. They were dielectric processes at very high frequencies and interfacial polarizations encountered in two phase systems. The latter dealt with the problem of electrical conductivity of polymers in relation to the technical application of certain polymers whose conductivity made possible their behaviour as semiconductors and, in some cases, even as conductors.

The subjects of the lectures given by HEIJBOER and by JOHNSON were, respectively, secondary loss maxima in glassy amorphous polymers and the effect of molecular weight distribution on physical properties of polymers.

Besides the corresponding lectures, each general subject attracted a number of scientific communications. In the first subject area about 110 communications dealt with radical and ionic polymerization and with polycondensation reactions. The 69 communications of the second subject could be sorted into several groups: degradation and stabilization of polymers; bulk and graft copolymers; and various reactions on polymers. On the third subject, 59 communications were presented; they developed work on the solid state, thermal transitions, crystallization, morphology, and solution properties of polymers. Finally, in the fourth subject area, the 47 communications dealt with flow properties, mechanical and dynamic properties, and thermal, electrical, optical, and magnetic properties, as well as the influence of additives on all these properties of polymers.

The reports of the IUPAC Working Parties were presented by J. MEISSNER ('Basic Parameters, Melt Rheology, Processing and End-use Properties of Three Samples of Low Density Polyethylene'), by J. L. S. WALES ('A Collaborative Study of Capillary Flow of a Highly Lubricated Unplasticized Polyvinylchloride'), and by C. L. STRAZIELLE ('Characterization of High Density and Low Density Polyethylene'). The Symposium main lectures and the Working Party report by MEISSNER will be published during 1975 in the IUPAC journal *Pure and Applied Chemistry* (scheduled Vol. 42, No. 4).

Prof. H. MARK animated the closing session with his very interesting lecture on 'New Polymer Events Worldwide'.

J. MILLAN

FORTHCOMING IUPAC-SPONSORED SYMPOSIA

I INTERNATIONAL MICROSYMPOSIUM ON POLYMERIZATION OF HETEROCYCLES (RING OPENING)

Jablonna, 23-25 June 1975

The Microsymposium is sponsored by the Macromolecular Division of IUPAC, and it will be organized jointly by the Centre of Molecular and Macromolecular Studies of the Polish Academy of Sciences (Lodz) and by the Centre of Macromolecular Research of CNRS (Strasbourg) under the auspices of the Polish-French Agreement for Scientific Cooperation. Jablonna is about 25 km from Warsaw. Accommodation is limited in Jablonna and some participants will be located in Warsaw.

Scientific Programme

The major part of the Microsymposium will consist of invited lectures, surveying the present state of knowledge concerning the Ring-opening Polymerization of Heterocycles, both anionic and cationic, with emphasis on the mechanisms of polymerization, on the preparation of models of biopolymers, and on biomedical polymers prepared by ring-opening polymerization processes. The following lecturers have kindly accepted to deliver the main presentations:

K. A. ANDRIANOV (USSR)
H. CHERDRON (FRG)
N. S. ENIKOLOPOV (USSR)
E. J. GOETHALS (Belgium)
V. A. KROPACHEV (USSR)
P. H. PLESCH (UK)
T. SAEGUSA (Japan)
P. SIGWALT (France)

G. SMETS (Belgium)
J. SEBENDA (Czechoslovakia)
J. SMID (USA)
M. SZWARC (USA)
T. TSURUTA (Japan)
E. VANDENBERG (USA)
O. VOGL (USA)

Their papers will be published in due course by IUPAC.

The number of participants will be kept sufficiently small to provide adequate conditions for detailed discussions. There will be no presentation of short communications. However, participants may submit contributions for the discussion sessions. The contributed papers should refer exclusively to domains covered by the Microsymposium and will be grouped into two sections, namely:

Kinetics and Mechanism of Ring-opening Polymerizations of Heterocyclic Monomers

Preparation of Models of Biopolymers and of Biomedical Polymers by Ring-opening Polymerization

There will be two discussion sessions, one for each series of contributed papers, and two panel discussions. All participants will receive the abstracts of contributed papers ahead of time, in order to get acquainted with their content prior to the discussion sessions.

Secretariat

For further information, please write to:

'Polymerization'
Polish Academy of Sciences
PL 90-362 Lodz
Poland

IV BRATISLAVA CONFERENCE ON POLYMERS MODIFIED POLYMERS, THEIR PREPARATION, AND PROPERTIES

Bratislava, 1-4 July 1975

This Conference is being organized under the sponsorship of IUPAC by the Polymer Institute of the Slovak Academy of Sciences, in cooperation with the Macromolecular Division of the Slovak Chemical Society and with the Department of Chemical Technology of Plastics and Fibres of the Slovak Technical University.

Scientific Programme

The scientific programme of the Conference will include the following fields:

Chemical and Physical Processes of Modification of the Molecular and Supermolecular Structure of Polymers

Properties of Modified Polymers in the Solid State and in Solution

These two topics will be covered by both main lectures and short communications. There will be no simultaneous sessions. So far main lectures have been kindly promised by:

N. F. BAKEEV (USSR)

Title not given

J. DOBÓ (Hungary)

Radiation-induced Changes in Polymeric Materials

H. INAGAKI (Japan)

Separation and Characterization of Block and Graft Copolymers by Thin Layer Chromatography

A. D. JENKINS (UK)

Synthesis of Graft Copolymers containing Acrylonitrile

N. A. PLATÉ (USSR)

Title not given

W. PRINS (USA)

Laser Light Scattering: A Probe for the Structure and Dynamics of Macromolecular Gels

G. REINISCH (GDR)

Formation of Microgels in Polymers by Thermal Activation

P. REMPP (France)

Recent Results on Chemical Modification of Polymers

The main lectures delivered at the Conference will be published in *Pure and Applied Chemistry*, the official journal of IUPAC.

Accommodation and Travel

Hotel accommodation will be available for all participants (single and double rooms). Foreign participants may arrive by plane either directly to Bratislava or via Prague (there is a regular air or train connection with Bratislava) or via Vienna by boat or bus.

Correspondence

All correspondence concerning the Conference should be addressed to:

Dr. A. ROMANOV
Polymer Institute
Slovak Academy of Sciences
Dúbravská Cesta
CS-809 34 Bratislava
Czechoslovakia

IX INTERNATIONAL CONGRESS OF CLINICAL CHEMISTRY

Toronto, 13-18 July 1975

The Congress is being organized by the Canadian Society of Clinical Chemists and the American Association of Clinical Chemists on behalf of the International Federation of Clinical Chemistry. It will include the 1975 annual scientific and business meetings of the Canadian and American Societies. All the activities of the Congress, including the Scientific Sessions and Technical Exhibition, will be centred at the Four Seasons Sheraton Hotel.

Plenary Session

The Immunological Revolution—R. A. GOOD (USA)
Future Areas of Activity for Clinical Chemistry—T. P. WHITEHEAD (UK)
International Clinical Chemistry—M. RUBIN (USA)

Symposia

Clinical Chemistry in Pediatrics

Homeostasis in the Neonate:

Respiratory Homeostasis—L. S. JAMES (USA)
Metabolic Homeostasis—G. CHANCE (Canada)

Genetic Metabolic Disease

Human Biochemical Genetics of Amino Acid Metabolism—C. R. SCRIVER (Canada)
Genetic Storage Diseases and Lysosomal Enzyme Defects—J. A. LOWDEN (Canada)

New Concepts in Interpretation of Laboratory Data—I

Trend and Cluster Analysis in Diagnosis and Prognosis of Myocardial Infarction—R. GRAMS (USA)
Statistical Approaches for Improved Use of Clinical Chemistry Data—P. WINKEL (Denmark)
Interpretation of Clinical Chemistry Data Using Electronic Data Processing—D. S. YOUNG (USA)
Individual and Group Variation—B. STATLAND (USA)

Primary Mechanisms of Hormone Action

Hormone Actions on Adenylate Cyclase Systems—M. RODBELL (USA)
The Mechanisms of Thyroid Hormone Action—J. OPPENHEIMER (USA)
Cellular Events Relating to the Action of Steroid Hormones—J. GRANT (UK)
Mechanisms of Action of Sex Steroids—E. BAULIEU (France)

New Concepts in Interpretation of Laboratory Data—II

Predictive Value of Laboratory Tests—R. GAMBINO (USA)

Time Dependent Variations in Laboratory Data: Diagnostic Use—D. STAMM (Federal Republic of Germany)

Reference Values in Human Chemistry—G. SIEST (France)

Metabolic Regulation

Molecular Strategy of Metabolic Regulation—G. WEBER (USA)

Regulation of Purine Metabolism in Man—J. B. WYNGAARDEN (USA)

Metabolic Regulation through Control of Enzyme Degradation—H. HOLZER (Federal Republic of Germany)

Control of Fuel Metabolism in Man—G. F. CAHILL (USA)

Control of Cholesterol Metabolism — Y. YAMAMURA (Japan)

Biochemical Aspects of Hyperalimentation

Hyperalimentation—S. DUDRICK (USA)

Metabolism of Endogenous and Exogenous Substrates during Intravenous Alimentation—J. P. FLATT (USA)

Biochemical and Nutritional Aspects of Fat Emulsions for Intravenous Use—A. WRETLIND (Sweden)

Amino Acid Metabolism in Intravenous Alimentation—H. ANDERSON (Canada)

Clinical Significance of Measurements of Drug Levels in Body Fluids

Drug Levels in Body Fluids as Indicators for Complications in Drug Therapy—E. J. ARIËNS (Netherlands)

The Pharmacological Rationale—Does Body Fluid Drug Analysis Provide a Reliable Basis for Therapeutic Control?—E. A. SELLERS (Canada)

Analytical Methodology—I. SUNSHINE (USA)

The Pharmacogenetic Aspects—What Do We Need to Know About the Individual in Order to Interpret the Data?—E. S. VESSEL (USA)

Reference Methods in Clinical Chemistry

This Symposium has been sponsored by IUPAC. The papers presented will be published in full in the journal *Pure and Applied Chemistry*.

Introduction—G. N. BOWERS (USA)

Rationale for Reference Methods—J. P. CALI (USA)

IFCC and Reference Methods—J. BUTTNER (Federal Republic of Germany)

A Reference Method for Glucose—R. SCHAFFER (USA)

Practical Applications of Reference Method Technology—F. L. MITCHELL (UK)

A Reference Method for Creatinine—S. H. JACKSON (Canada)

Immunology Interrelations with Clinical Chemistry

Standardization of Quantitation of the Immunoglobulins—D. S. ROWE (Switzerland)

Principles and Problems of Radioimmunoassays—L. P. CAWLEY (USA)

Carcinoembryonic Antigens—N. ZAMCHECK (USA)

Cellular and Enzymatic Basis of Immunological Deficiency Diseases—F. COHEN (USA)

Emerging High Sensitivity Analytical Techniques

Clinical Mass Spectrometry—M. G. HORNING (USA)

Advances in Centrifugal Fast Analyzer Development—C. A. BURTIS (USA)

The Future of High Resolution Techniques in the Clinical Laboratory—E. JELLUM (Norway)

Clinical Applications of Enzyme-linked Immunoassay Techniques—
B. WISDOM (Ireland)
Microcalorimetry in Clinical Chemistry—K. LEVIN (Sweden)

Diagnostic Biochemistry and Tissue Culture

Diagnosis of Mucopolysaccharidoses and Mucolipidoses in Cultured Fibroblasts—E. NEUFELD (USA)
Investigation of Chondrodystrophies Using Cultured Chondrocytes—
D. W. HOLLISTER (USA)
Carrier Detection in X-Linked Disease Using Cloned Cell Cultures—
M. W. SPENCE (Canada)
Ultramicroassays of Enzyme Activities of Single Cultured Cells—P. HOSLI (Netherlands)

Clinical Chemistry—Perspectives of a Changing Discipline

Perspectives of Clinical Chemistry as Seen From the Hospital Laboratory—
J. H. WILKINSON (UK)
Perspectives of Clinical Chemistry as Seen From the Independent Laboratory—
R. J. HENRY (USA)
Perspectives of Clinical Chemistry as a Changing Research Discipline—
P. ASTRUP (Denmark)
Future Education and Training Requirements of Clinical Biochemists—
A. G. GORNALL (Canada)

Contributed Papers

Contributed papers will be presented in four simultaneous meetings during the afternoons. In addition to the oral presentations, poster sessions will also be arranged each afternoon. Abstracts of the papers to be presented will be published in the June 1975 issue of *Clinical Chemistry* in the form in which they are submitted by the authors. The abstracts will also be distributed to delegates at the time of registration.

Secretariat

For further information, please write to the following address:

IX International Congress of Clinical Chemistry
Toronto Dominion Centre
POB 34, Toronto
Ontario MK5 1B7
Canada

**XV PRAGUE MICROSYMPOSIUM ON
MACROMOLECULES DEGRADATION AND
STABILITY OF POLYOLEFINS**

Prague, 21-24 July 1975

Scientific Programme

Mechanisms of Degradation Processes

(a) Mechanism and kinetics of elementary reactions taking part in degradation processes and caused by thermal treatment, oxygen, and irradiation and/or by combinations of those influences. Energetic relations, transformations of energy.

(b) Chemistry and structure of polyperoxides, products of transformations.

(c) Influence of the chemical structure and morphology of polyolefins on the mechanism of degradation processes. Modification of inherent resistance and sensitivity of PE and PP against degradation and atmospheric ageing.

Characterization of Degradation and Stabilization Processes

Methods for comparison of the course and extent of degradation processes under conditions of atmospheric natural and accelerated ageing. Limitations of correlation factors; differences in mechanism of elementary degradation processes.

Stabilization Systems and their Chemical Transformations

(a) Stabilization systems against individual degradation processes; combination of systems and their mutual interactions; activity of mixtures of stabilizers.

(b) Interactions and chemical transformation processes in the system polyolefin-stabilizer; influence of products of transformation of stabilizers; physical interactions (compatibility, migration, volatility of stabilizers).

Time-controlled and Limited Stabilization

Chemical and physical bases for preparation of polymers with controlled lifetime (photo- and biodegradable polymers).

The aim is a discussion of the complex relationships dealing with polyolefins in connection with atmospheric ageing, thermooxidative changes, and mechanical treatment. Main interest will be devoted to various degradation processes and new trends in influencing those processes by additives or by chemical modifications of the polymeric chain to obtain polyolefins having properties fitting required technical applicability as well as environmental control.

The scientific sessions will consist of invited lectures, short communications, and panel discussions. The main lectures will provide a broad survey of recent developments. The following speakers have been invited: N. C. BILLINGHAM (UK), H. P. FRANK (Austria), J. E. GUILLET (Canada), W. L. HAWKINS (USA), H. NAARMANN (FRG), M. SCHULZ (GDR), G. SCOTT (UK), and two lecturers from USSR.

Four panel discussions related to individual topics should allow confrontation of views on mechanisms and limitations taking place in the degradation and stabilization of polyolefins. English is preferred for all Microsymposium contributions. For Russian speaking participants, the necessary interpreting will be provided during discussions.

Other Information

All sessions will be held in the Institute of Macromolecular Chemistry of the Czechoslovak Academy of Sciences in Prague. Social events and a ladies programme are planned. Further information with final registration forms is available from:

XV Prague Microsymposium
PMM Secretariat
c/o Institute of Macromolecular Chemistry
Czechoslovak Academy of Sciences
CS-162 06 Prague 616 - Petřiny
Czechoslovakia

IV INTERNATIONAL SYMPOSIUM ON CAROTENOIDS

Berne, 25-29 August 1975

The Symposium will be held in the building of the University Institute of Inorganic Chemistry.

Session Lectures

The Session Lecturers will give a selective review (45 minutes) on their topic covering the period 1970-75 and include the work of other groups. Selected Session Lectures will be published in *Pure and Applied Chemistry*, official journal of IUPAC, and also made available as a special bound reprint.

Physical Methods

G. P. MOSS	NMR-Spectroscopy
W. KLYNE <i>et al.</i>	Circular Dichroism

Complexed Carotenoids

P. F. ZAGALSKY <i>et al.</i>	Carotenoproteins
H. PFANDER	Glycosides

Structure, Stereochemistry

S. LIAAEN-JENSEN	New Structures
J. SZABOLCS	

Synthesis and Reactions

B. C. L. WEEDON	Synthesis
S. M. MAKIN	Dienol Ether Synthesis

Technology (including Vitamin A)

F. KIENZLE <i>et al.</i>	Technology
O. WISS	Vitamin A
G. ZBINDEN	Toxicology

Degradation Products

J. D. BU'LOCK	Trisporic Acid
R. S. BURDEN <i>et al.</i>	ABA/Xanthoxin

Biochemistry

B. H. DAVIES	Primary Steps of Biosynthesis
G. BRITTON	Final Steps of Biosynthesis
W. RAU	Photoinduction
T. W. Goodwin	Closing remarks

The scientific programme will also include a number of contributed papers (30 minutes).

Correspondence

Correspondence should be addressed to:

Dr. H. PFANDER, Secretary General
IV International Symposium on Carotenoids
University Institute of Organic Chemistry
Länggass-Strasse 7, CH-3012 Berne
Switzerland

SYMPOSIUM ON EDUCATIONAL TECHNOLOGY IN THE TEACHING OF CHEMISTRY

Madrid, 6-7 September 1975

Organized by the IUPAC Committee on Teaching of Chemistry, the Symposium will review trends in the use of educational technology in the teaching of chemistry at secondary and tertiary levels, and will attempt to evaluate the use of educational techniques.

The following programme of main lectures is being arranged:

Developments in the Tools of Educational Technology in the Last Decade	W. T. LIPPINCOTT (USA)
Educational and Other Factors Affecting Selection of Techniques for Effective Teaching	M. J. FRAZER (UK)
Mass Media and Chemical Education	L. J. HAYNES (UK)
Effectiveness of Tools of Modern Educational Technology in Teaching of Chemistry in the Classroom and Laboratory	I. V. BEREZIN (USSR)
Computer-assisted Instruction in Chemical Education	A. KORNHAUSER (Yugoslavia)
Programmed Learning in Chemistry: Where do Computers come in?	J. A. YOUNG (USA)
Educational Technology in the Developing Countries: Problems and Challenges	R. C. MEHROTRA (India) A. GUERRERO (Argentina)
International Cooperation in Educational Technology	C. N. R. RAO (India)

The Symposium will be completed with a session in which National Representatives from the Committee on Teaching of Chemistry make brief presentations (10 minutes) on educational technology in their respective countries.

Further Information

For further details about the Symposium, please write to:

Trans World Conference Organisers Ltd.
23-25 Procter Street
London WC1V 6LD, UK

INTERNATIONAL SYMPOSIUM ON MARINE NATURAL PRODUCTS

Aberdeen, 8-11 September 1975

This Symposium, sponsored by the Perkin Division of the UK Chemical Society and IUPAC, will be concerned with the structure, chemistry, and biosynthesis of metabolites from marine animals and plants.

Invited Lecturers

J. T. BAKER (Sydney), P. J. SCHEUER (Hawaii), D. J. FAULKNER (La Jolla), B. TURSCH (Brussels), L. MINALE (Naples), A. J. WEINHEIMER (Oklahoma).

The invited lectures will be published in *Pure and Applied Chemistry*, the official journal of IUPAC. Abstracts of contributed papers will be circulated in advance to registered participants.

Registration and Accommodation

Advance registration for attendance at the meeting is required. Accommodation for registered participants will be available in a modern hall of residence at the University of Aberdeen, where the scientific sessions will also be held. For further information, please write to:

Dr. J. F. GIBSON
Chemical Society
Burlington House
Piccadilly
London W1V 0BN, UK

XVIII COLLOQUIUM SPECTROSCOPICUM INTERNATIONALE

Grenoble, 15-19 September 1975

The Colloquium is being organized, under the sponsorship of IUPAC, by Groupement pour l'Avancement des Méthodes Spectroscopiques et Physico-chimiques d'Analyse (GAMS). Grenoble, the economic and intellectual capital of the French Alps, is a city set amongst magnificent mountains. It gives the conference the important assets of hotel accommodation and opportunity of tourism, as well as the notable facilities of the campus of the University of Saint Martin d'Hères.

Scientific Programme

The area covered includes all the branches of spectroscopy, in particular:

- spectroscopy of electromagnetic radiations (emission, absorption, fluorescence, diffraction)
- spectroscopy of particles (mass spectroscopy, photoelectron spectroscopy, ESCA)
- γ -ray spectroscopy, Mössbauer spectroscopy
- nuclear magnetic resonance, electron spin resonance
- molecular spectroscopy (IR, UV, visible, Raman)

The programme includes primary analysis as well as structural analysis, concerning molecules or more complex environments, such as solids. There will be plenary lectures, sessional lectures, round table discussions, and papers. An instrument exhibition will be held, as well as technical visits. The topics selected for the round table discussions are:

- trace analysis in mineral and geological samples
- analysis of surfaces
- interactions in flameless atomic absorption
- applications of molecular spectroscopy to determination of organic structures

Complimentary Programme

Technical visits, a cultural and tourist programme, and a programme for ladies will be provided. For further information, please write to:

Monsieur le Directeur du GAMS
XVIII CSI
10 Rue du Delta
F-75009 Paris, France

INTERNATIONAL CONFERENCE ON COLLOIDS AND SURFACES

San Juan, Puerto Rico, 21-25 June 1976

The Division of Colloid and Surface Chemistry of ACS and IUPAC are sponsoring this meeting on the occasion of the 50th anniversary of the founding of the Division and the 50th National Colloid Symposium.

Scientific Programme

This will consist of plenary lectures, invited lectures, and contributed papers. The following plenary lectures will be delivered:

Rheology of Disperse Systems	S. G. MASON (Canada)
Atomic and Molecular Processes at Solid Surfaces	G. SOMORJAI (USA)
Aerosol Science and Atmospheric Physics	M. KERKER (USA)
Membranes	J. F. DANIELLI (USA)
Stability and Instability in Disperse Systems	R. H. OTTEWILL (UK)
Liquid Crystals	G. H. BROWN (USA)
Catalysis	R. L. BURWELL (USA)
Surface Thermodynamics	I. PRIGOGINE (Belgium)
Water at Interfaces	F. FRANKS (UK)
Forces at Interfaces	D. TABOR (UK)

Further Information

Those persons wishing to receive further information or contribute a paper should contact:

MILTON KERKER
Clarkson College of Technology
Potsdam, New York 13676
USA

V INTERNATIONAL FERMENTATION SYMPOSIUM

Berlin (West), 28 June-3 July 1976

The Symposium will take place in the Berlin Congress Hall. It is being sponsored by the Fermentation Section of IUPAC and supported by the Bundesminister für Forschung auf Technologie, by the Senat von Berlin and the German Fermentation Industries. There will be cooperation with the DECHEMA Deutsche Gesellschaft für Chemisches Apparatewesen eV, Deutsche Gesellschaft für Hygiene und Mikrobiologie eV, Gesellschaft für Biologische Chemie, and Gesellschaft Deutscher Chemiker.

Scientific Programme

The scientific programme will include plenary lectures by invited speakers and short presentations of recent results covering the following topics:

Fermenter Operations
Instrumentation for Process Control
Process Design and Product Recovery
Mass and Energy Transfer and Scalingup
Growth Kinetics and Mathematical Models

Continuous Culture

Fermentation of Hydrocarbons and Unconventional Substrates

Metabolic Regulation and Physiological Fundamentals of Industrial Microorganisms

Isolation and Maintenance of Industrial Useful Strains

Genetics Applied to Process Improvement

Microbial Biomass Production

Improvements of Known Fermentation Processes

New Microbial Products and Processes

Microbial Enzymes of Industrial Interest

Immobilized Enzymes

Tissue Cell Culture

Transformation of Compounds by Microorganisms

Improved Microbial Waste and Sewage Treatment

Recent Progress in Traditional Food Production by Fermentation

New Aspects in Brewing and Distilling

Education in Biochemical Engineering

Standardization of Fermentation Terminology

Equipment and Raw Materials

Patents and Strain Deposition

The official languages will be English, French, and German. However, all papers should be presented in English if possible. Abstracts of papers will be published in English.

Correspondence

All correspondence concerning the Symposium should be addressed to:

Secretariat V International Fermentation Symposium

c/o Institut für Gärungsgewerbe

und Biotechnologie

Seestrasse 13

D-1000 Berlin 65

Federal Republic of Germany

IUPAC SECRETARIAT STAFF CHANGE

Mr. R. J. M. RATCLIFFE relinquished his position as Assistant Secretary at the end of February. Through his new organization, Trans World Conference Organisers Ltd., he hopes to provide appropriate services for various national and international bodies. His successor at the IUPAC Secretariat is Miss A. TROUGHTON, who was previously with Pergamon Press Ltd.

CRITICAL SURVEYS OF STABILITY CONSTANTS OF METAL COMPLEXES

GUIDELINES FOR PROSPECTIVE AUTHORS

Critical Surveys of Stability Constants of Metal Complexes is a continuous series, edited by the IUPAC Commission on Equilibrium Data. Each Critical Survey will be published in the official journal of IUPAC, *Pure and Applied Chemistry*, enabling the series to be bound at a later date in a more permanent, hard-cover volume. The aim of the series is to evaluate the most reliable equilibrium constants from the available and frequently conflicting data.

Each survey is prepared by an expert, working actively in the field of thermodynamics of complexes. The papers are normally written by solicited authors. Unsolicited authors should first send an outline of their intended survey to avoid parallel work. Each survey, written by either solicited or unsolicited authors, is circulated among and commented on by the Members of the Commission on Equilibrium Data. It follows from the nature of the data considered, however, that even the recommended values cannot be regarded as 'official' ones and further research may change the suggestion.

In a Critical Survey reference should be made to all published data, but the numerical values should not necessarily be mentioned. The data are handled in four categories: recommended, tentative, doubtful, rejected. It must definitely be stated why certain data are rejected and particularly why certain data are regarded as reliable.

- (a) Data should be *recommended* if the results of at least two independent groups are available and they are in good agreement; if the surveyor has no doubt as to the adequacy of the applied experimental and calculation procedure; if the consideration of the activity-concentration relation is correct and the standard state is unambiguous. The given error of such a constant must be less than ± 0.05 logarithmic unit.
- (b) Data should be regarded as *tentative* if all the conditions mentioned in connexion with the *recommended* category are fulfilled, except the first, or if the surveyor observes some deviation from the necessary rigorousness, but this probably caused no serious mistakes. The given error of such a constant cannot exceed ± 0.2 logarithmic unit.
- (c) Data should be considered as *doubtful* if the surveyor found some mistake in the evaluation of the constants, which are nevertheless of semiquantitative value. The probable error of such a constant should not exceed ± 1 logarithmic unit.
- (d) Data determined by an inadequate method, or obtained under undefined conditions, or where any serious objection is found in the evaluation, should be *rejected*.

Only *published* data should be included in the surveys. Quotations such as 'unpublished data', 'personal communication', *etc.*, should be omitted. Even the published data can be considered only if the presented experimental details permit assessment of the degree of reliability of the constants.

A Critical Survey should preferably be written on the different complexes of a certain ligand or family of ligands, although in certain cases other groupings are accepted (*e.g.*, complexes of a certain metal ion or a family of metal ions). Besides stability constants, ΔH and ΔS data should be included where available. For these data the same rules should be applied as for the equilibrium constants.

Arrangement of the Paper

Although strict uniformity in the format of papers is not expected, the following rules should be followed.

1. In the Introduction, the general characterization of the treated ligand (or metal ion) and of the complexes should be given. Stress should be laid on the problems connected with the determination of the stability constants, for the particular ligand.
2. The order of metal ions should follow the order applied in the volumes of *Stability Constants of Metal-Ion Complexes*, inorganic section, independently of whether the ligand in question is organic or inorganic. When a family of ligands is considered, it is suggested that the data be treated in an order permitting meaningful comparison.
3. To conclude the consideration of the constants referring to a certain equilibrium or set of equilibria, a constant or set of constants should be given, indicating the degree of reliability. In doing this the rules mentioned above should be applied.
4. Although a low degree of reliability is an immediate indication of the subjects requiring further work, it is suggested that fields be indicated where further careful studies are particularly desirable.
5. The reference numbers should be given in parentheses in the text or in the tables. The same bibliographic system should be applied as in *Stability Constants*; the last two digits of the year of publication and the initial of the family name of the first author. A list of references should be given in alphabetical order at the end of the paper.
6. All manuscripts should be sent in duplicate to the Chairman of the Commission on Equilibrium Data, who is at present:

Prof. G. N. NANCOLLAS
Department of Chemistry
State University of New York
Acheson Hall
Buffalo, New York 14214
USA

or to the Project Leader, who is at present:

Prof. M. T. BECK
Institute of Physical Chemistry
Kossuth Lajos University
H-4010 Debrecen
Hungary

Surveys Received

The following Critical Surveys have been compiled and are at present being prepared for publication by the Commission on Equilibrium Data:

Survey on EDTA Complexes	G. ANDEREGG
Survey on Cyano Complexes	M. BECK
Critical Evaluation of Some Equilibrium Constants involving Alkylammonium Extracts	A. S. KERTES

NEW APPENDICES TO IUPAC INFORMATION BULLETIN

Readers are reminded that IUPAC nomenclature recommendations are first issued in provisional form. A minimum period of 8 months is allowed for receipt of comments on such recommendations from throughout the world. This helps to ensure that when revised recommendations are published eventually in *Pure and Applied Chemistry*, they will be acceptable to and used by the international chemical community.

The following new *Appendices on Provisional Nomenclature, Symbols, Units, and Standards* were issued in January 1975:

- No. 41 Chemical Nomenclature, and Formulation of Compositions, of Synthetic and Natural Zeolites (Commission on Nomenclature of Inorganic Chemistry and Commission on Colloid and Surface Chemistry in collaboration with International Mineralogical Association)
- No. 42 Recommendations for Sign Conventions and Plotting of Electrochemical Data (Commission on Electroanalytical Chemistry)
- No. 43 Recommendations for Nomenclature of Ion-selective Electrodes (Commission on Analytical Nomenclature)
- No. 44 Recommendations for Publication of Papers on Molecular Absorption Spectrophotometry in Solution between 200 and 800 nm (Commission on Analytical Nomenclature)

Gratis copies may be obtained by writing to:

Assistant Secretary (Publications)
IUPAC Secretariat
Bank Court Chambers
2-3 Pound Way
Cowley Centre
Oxford OX4 3YF, UK

Subscribers to the *Information Bulletin* receive all Appendices automatically and free-of-charge on publication. For Appendices issued earlier, see *Information Bulletin* No. 48 (October 1974, page 128).

Subject to the prior agreement of IUPAC, its provisional nomenclature recommendations may be:

- (a) Republished in other journals.
- (b) Translated into other languages through National Adhering Organizations.

MISCELLANEOUS PUBLICATIONS

PRIMARY PUBLICATIONS AND SECONDARY SERVICES: PARTNERS IN INFORMATION FLOW

This book contains the papers presented at a Conference arranged by the ICSU Abstracting Board in cooperation with the Royal Society (London, July 1973), where problems of mutual concern to primary editors and secondary services were discussed.

Primary publications are, so to speak, the substrate on which the secondary services feed. Until recently, however, the interest has been a kind of one-way traffic, in which the secondary services and other interested bodies, particularly UNESCO and the scientific unions constituting ICSU, have addressed a series of exhortations to the editors of primary publications on how they should conduct their journals. About 1970 ICSU AB realized the ineffectiveness of this approach to matters of mutual concern, and initiated a programme of encouraging close contact and cooperation between primary publications and abstracting and indexing services. This programme has consisted of two main parts: a Joint Working Group consisting of representatives of Associations of Editors of primary publications and of ICSU AB, and a series of open meetings at which problems of common interest were discussed.

The present Conference is the most ambitious of the series of meetings. In addition to continuing the dialogue on matters like titles, abstracts, bibliography, and indexing, the programme is arranged to give editors of primary publications, especially of scientific and technological journals, an insight into the problems and methods of working of modern abstracting and indexing services.

This book is available from the ICSU AB Secretariat, 17 Rue Mirabeau, F-75016 Paris, France: price US\$ 18 plus mailing charges.

NEW PUBLICATIONS FROM INTERNATIONAL UNION OF CRYSTALLOGRAPHY

Structure Reports

Strenuous efforts have been made by the Chairman and Members of the IUCr Commission on Structure Reports, to bring this extensively used set of volumes up to date. For Volume 30 (covering the literature for 1965) onwards, *Structure Reports* has been divided into two parts: Part A. Metals and Inorganic Compounds, and Part B. Organic Compounds (including organometallic compounds).

The first five new Parts were published towards the end of 1974. They are Volumes 30B, 31B, 32B, 33B, and 35B, and cover the literature on organic compounds for the years 1965-1968 inclusive and 1970. The volume for 1963, which is the only remaining volume in which reports on all three sections will appear in one bound book, was published early in 1975. The remaining volumes covering all the literature up to the end of 1970 should be published during 1975.

Published for IUCr by Oosthoek, Scheltema & Holkema, Emmalaan 27, Utrecht, Netherlands.

International Tables for X-Ray Crystallography

Volume IV, containing revised and supplementary tables to Volumes II and III, was published in 1974. It contains revised values for atomic scattering factors, X-ray wavelengths, and atomic absorption coefficients. At the same time a number of special topics not included in Volume II have been included in the new volume. Much of the revised material supersedes corresponding material in the earlier volumes and Volume IV should always be consulted first. It contains a cumulative index for all four volumes.

Published for IUCr by Kynoch Press, Birmingham, UK.

Proceedings of Inter-Congress Conference on Anomalous Scattering (Madrid, 22-26 April 1974)

This is the first book to be devoted entirely to the important subject of anomalous scattering of X-rays and neutrons. It contains 33 invited papers presented at the Conference which was organized by the IUCr Commission on Crystallographic Apparatus. The papers are arranged in eight chapters on theoretical calculation and experimental determination of dispersion corrections, novel applications of anomalous scattering, absolute configuration and tensorial properties, accurate intensity measurement, effects of dispersion on atomic parameters, use of anomalous scattering in protein structure analysis, and structure determination using neutron anomalous scattering. Each chapter concludes with a narrative account of the lively discussion in that session.

This extensively indexed book (about 550 pp.) will be of immediate and continued value to all who measure and make use of anomalous scattering, whether in structural investigations, in solid-state physics, or in X-ray diffraction physics. It is edited by S. RAMASESHAN and S. C. ABRAHAMS, with a foreword by the President of the Union.

The book is being printed in Parma and published for the Union by Munksgaard, in Copenhagen, from whom copies may be ordered. Orders may also be placed with Polycrystal Book Service or any bookseller. Copies will be available in about March 1975, at a cost of 200 Danish Kroner, currently equivalent to about \$35 or £15.

CALENDAR OF IUPAC-SPONSORED MEETINGS

	1975	
June 2-6	V International Conference on Atomic Masses and Fundamental Constants (AMCO-5 Secrétariat, Institut d'Electronique Fondamentale, Bat. 220—Université Paris-Sud, F-91405 Orsay, France)	Paris (France)
June 16-19	I Symposium International sur la Chimie Heterocyclique Minerale (ou Inorganique) (Prof. H. GARCIA-FERNANDEZ, Laboratoire d'Electrochimie, Faculté des Sciences, F-25030 Besancon, France)	Besancon (France)
June 23-25	International Microsymposium on Polymerization of Heterocycles: Ring Opening ('Polymerization', Polish Academy of Sciences, PL 90-362 Łódź, Poland)	Jablonna (Poland)
July 1-4	XII European Congress of Molecular Spectroscopy (Prof. M. GROSMAUN, Secretary of Organizing Committee, XII European Congress of Molecular Spectroscopy, Laboratoire de Spectroscopie et d'Optique du Corps Solide, Université Louis Pasteur Strasbourg I, 5 Rue de l'Université, F-67000 Strasbourg, France)	Strasbourg (France)
July 1-4	IV Bratislava Conference on Polymers: Modified Polymers. Their Preparation and Properties (Dr. A. ROMANOV, Chairman of Organizing Committee, IV Bratislava Conference on Polymers, Polymer Institute, Slovak Academy of Sciences, Dúbravská Cesta, CS-809 34 Bratislava, Czechoslovakia)	Bratislava (Czechoslovakia)
July 6-11	25th IUPAC Congress (Organizing Committee, 25th IUPAC Congress, POB 983, Jerusalem, Israel)	Jerusalem (Israel)
July 13-18	International Symposium on Macromolecules (Secretariat, IUPAC Symposium on Macromolecules, Aharon Katzir-Katchalsky Center, Weizmann Institute of Science, Rehovot, Israel)	Jerusalem (Israel)
July 13-18	IX International Congress of Clinical Chemistry (Secretariat, IX International Congress of Clinical Chemistry, Toronto Dominion Centre, POB 34, Toronto, Ontario MK5 1B7, Canada)	Toronto (Canada)
July 21-24	XV Prague Microsymposium on Macromolecules: Degradation and Stabilization of Polyolefins (XV Prague Microsymposium, PMM Secretariat, c/o Institute of Macromolecular Chemistry, Czechoslovak Academy of Sciences, CS-162 06 Prague 616—Petržiny, Czechoslovakia)	Prague (Czechoslovakia)
August 25-29	IV International Symposium on Carotenoids (Dr. H. PFANDER, Secretary General of Organizing Committee, IV International Symposium on Carotenoids, University Institute of Organic Chemistry, Länggass-Strasse 7, CH-3012 Berne, Switzerland)	Berne (Switzerland)
August 26-30	IV International Conference on Chemical Thermodynamics (Prof. M. LAFFITTE, Chairman of Organizing Committee, IV International Conference on Chemical Thermodynamics, Centre de Recherches de Microcalorimétrie de et Thermochimie, Centre National de la Recherche Scientifique, 26 Rue du 141° RIA, F-13003 Marseille, France)	Montpellier (France)
September 2-11	28th IUPAC Conference: closed meeting of IUPAC bodies (Executive Secretary IUPAC, IUPAC Secretariat, Bank Court Chambers, 2-3 Pound Way, Cowley Centre, Oxford OX4 3YF, UK)	Madrid (Spain)
September 8-11	International Symposium on Marine Natural Products (Dr. J. F. GIBSON, International Symposium on Marine Natural Products, Chemical Society, Burlington House, Piccadilly, London W1V 0BN, UK)	Aberdeen (UK)

September 12-16	Round Table on Study and Applications of Transport Phenomena in Thermal Plasmas (Prof. M. FOEX, Laboratoire des Ultra-Réfractaires, Centre National de la Recherche Scientifique, BP 5, Odeillo, F-66120 Font Romeu, France)	Font Romeu (France)
September 15-19	XVIII Colloquium Spectroscopicum Internationale (Monsieur le Directeur du GAMS, XVIII CSI, 10 Rue du Delta, F-75009 Paris, France)	Grenoble (France)
September 15-20	International Conference on Colloid and Surface Chemistry (Prof. E. WOLFRAM, Secretary of Organizing Committee, International Conference on Colloid and Surface Chemistry, Department of Colloid Science, Loránd Eötvös University, Puskin U. 11-13, H-1088 Budapest, Hungary)	Budapest (Hungary)
September 18-23	International Symposium on Plasma Chemistry (Prof. H. SUHR, Chemisches Institut der Universität Tübingen, Auf der Morgenstelle, D-7400 Tübingen 1, Federal Republic of Germany)	Rome (Italy)
October 27-31	III International Symposium on Bioelectrochemistry (Prof. H. W. NÜRNBERG, Institut für Angewandte Physikalische Chemie der Kernforschungsanlage Jülich GmbH, Postfach 365, D-5170 Jülich, Federal Republic of Germany)	Jülich (Federal Republic of Germany)
1976		
June 21-25	International Conference on Colloids and Surfaces (MILTON KERKER, Clarkson College of Technology, Potsdam, New York 13676, USA)	San Juan (Puerto Rico)
June 28 -July 3	V International Fermentation Symposium (V International Fermentation Symposium, Institut für Gärungsgewerbe und Biotechnologie, Seestrasse 13, D-1000 Berlin 65, Federal Republic of Germany)	Berlin (Federal Republic of Germany)
July 12-16	VI International Congress on Catalysis (Dr. J. F. GIBSON, VI International Congress on Catalysis, Chemical Society, Burlington House, Piccadilly, London W1V 0BN, UK)	London (UK)
August 16-21	VIII International Symposium on Carbohydrate Chemistry (Prof. K. ONODERA, Department of Agricultural Chemistry, Kyoto University, Kyoto, Japan)	Kyoto (Japan)
August 23-28	X International Symposium on Chemistry of Natural Products (Mr. L. C. SOMERVILLE, Royal Society of New Zealand, 6 Halswell Street, POB 12-249, Wellington, New Zealand)	Dunedin (New Zealand)
September	III IUPAC Conference on Physical Organic Chemistry (Prof. G. LAMATY, Laboratoire de Chimie Organique Physique, Université des Sciences et Techniques du Languedoc, Place Eugène Bataillon, F-34060 Montpellier Cedex, France)	Montpellier (France)
1977		
July 18-23	XVIII International Conference on Coordination Chemistry (Prof. P. SENISE, Chairman of Organizing Committee, XVIII International Conference on Coordination Chemistry, Instituto de Química, Universidade de São Paulo, Caixa Postal 20780, São Paulo, Brazil)	São Paulo (Brazil)
September 4-10	26th IUPAC Congress (Prof. T. ASAHARA, Chairman of Preliminary Organizing Committee, Science Council of Japan, 22-23 Roppongi 7-chome, Minato-ku, Tokyo 106, Japan)	Tokyo (Japan)

CALENDAR OF NON-IUPAC MEETINGS

1975

April 2-4	Colloque International sur les Matériaux de Substitution pour les Composants Électroniques (Secrétariat du Colloque, 16 Rue de Presles, F-75740 Paris Cedex 15, France)	Paris (France)
April 7-11	Annual Chemical Congress of Chemical Society and Royal Institute of Chemistry (Dr. J. F. GIBSON, Chemical Society, Burlington House, Piccadilly, London W1V 0BN, UK)	York (UK)
April 8-16	Symposium on Advances in Industrial Nitration Chemistry (Prof. L. F. ALBRIGHT, School of Chemical Engineering, Purdue University, Lafayette, Indiana 47907, USA; and Prof. C. HANSON, School of Chemical Engineering, University of Bradford, Bradford BD7 1DP, Yorkshire, UK)	Philadelphia (USA)
April 8-11	Reaktortagung 1975 (Deutsches Atomforum eV, Allianplatz, Haus X, D-5300 Bonn 1, Federal Republic of Germany)	Nürnberg (Federal Republic of Germany)
April 16-17	Application of Chemical Engineering to Treatment of Sewage and Industrial Liquid Effluents (Dr. D. GELDART, School of Chemical Engineering, University of Bradford, Bradford BD7 1DP, Yorkshire, UK)	York (UK)
May 5-7	I International Congress on Polymer Concretes [The Concrete Society (Congress), Terminal House, Grosvenor Gardens, London SW1W 0AJ, UK]	London (UK)
May 11-16	147th Meeting of Electrochemical Society (Mr. V. H. BRANNEY, Assistant Executive Secretary, Electrochemical Society Inc., POB 2071, Princeton, New Jersey 08540, USA)	Toronto (Canada)
May 26-28	58th Canadian Chemical Conference and Exhibition of Chemical Institute of Canada (Chemical Institute of Canada, 151 Slater Street, Suite 906, Ottawa, Ontario K1P 5H3, Canada)	Toronto (Canada)
May 26-30	Colloque International sur l'Électronique et la Mesure (Secrétariat du Colloque, 16 Rue de Presles, F-75740 Paris Cedex 15, France)	Paris (France)
June 10-13	International Symposium on Chemurgy of Fats (Dr. W. ZWIERZYKOWSKI, Instytut Chemii i Technologii Organicznej oraz Żywnościowej, Politechnika Gdańska, Ul. Majakowskiego 11, PL 80-952 Gdańsk, Poland)	Gdańsk (Poland)
June 16-18	Symposium on High Temperature Chemical Reaction Engineering (N. T. SHEPHERD, Institution of Chemical Engineers, 15 Belgrave Square, London SW1X 8PT, UK)	Harrowgate (UK)
June 17-20	27th International Meeting of Société de Chimie Physique: Lasers in Physical Chemistry (Dr. C. TROYANOWSKY, General Secretary, Société de Chimie Physique, 10 Rue Vauquelin, F-75231 Paris Cedex 05, France)	Paris (France)
June 18-20	Colloque International sur la Fiabilité et la Disponibilité des Systèmes Informatiques (Secrétariat du Colloque, 16 Rue de Presles, F-75740 Paris Cedex 15, France)	Paris (France)

June 24– July 3	IV International Summer Conference: Chemistry of Solid-Liquid Interfaces (Dr. V. PRAVDIC, Rudjer Bošković Institute, POB 1016, YU-41001 Zagreb, Yugoslavia)	Cavtat-Dubrovnik (Yugoslavia)
June 26–27	DECHEMA-1975 (DECHEMA, Theodor-Heuss-Allee 25, Postfach 970146, D-6000 Frankfurt/Main 97, Federal Republic of Germany)	Frankfurt/Main (Federal Republic of Germany)
July 6–11	III International Meeting on NMR Spectroscopy (Dr. J. F. GIBSON, Chemical Society, Burlington House, Piccadilly, London W1V 0BN, UK)	St. Andrews (UK)
July 14–17	IV International Symposium on Synthesis in Organic Chemistry (Dr. J. F. GIBSON, Chemical Society, Burlington House, Piccadilly, London W1V 0BN, UK)	Cambridge (UK)
July 27– August 1	Gordon Conference on Photochemistry (Dr. A. A. BELL, Bell Telephone Laboratories Inc., 600 Mountain Avenue, Murray Hill, New Jersey 07974, USA)	Tilton New Hampshire (USA)
July 29– August 6	International Conference on Improvement of Physics Education (Dr. R. M. SILLITTO, Department of Physics, University of Edinburgh, Mayfield Road, Edinburgh, UK)	Edinburgh (UK)
August 7–12	VIII International Conference on Photochemistry (Prof. O. P. STRAUZ, Department of Chemistry, University of Alberta, Edmonton, Alberta T6G 2E1, Canada)	Edmonton (Canada)
August 7–15	X General Assembly and International Congress of Crystallography (Congress Organizing Committee, POB 7205, Amsterdam, Netherlands)	Amsterdam (Netherlands)
August 24–29	5th International Congress of Chemical Engineering, Chemical Equipment, Design, and Automation (Secretariat, 5th CHISA-Congress, POB 857, Praha 1, Czechoslovakia)	Prague (Czechoslovakia)
August 25–30	II European Conference on Analytical Chemistry (EUROANALYSIS II, c/o Hungarian Chemical Society, POB 240, H-1368 Budapest, Hungary)	Budapest (Hungary)
August 25–29	V International Conference on Atomic Spectroscopy (Dr. J. B. WILLIS, Secretary, V International Conference on Atomic Spectroscopy, CSIRO Division of Chemical Physics, POB 160, Clayton, Victoria, Australia 3168)	Clayton-Melbourne (Australia)
August 25– September 6	XVI General Assembly of International Union of Geodesy and Geophysics (Comité National Français de Géodésie et Géophysique, 136 bis, Rue de Grenelle, F-75700 Paris, France)	Grenoble (France)
September 1–3	6th Symposium on Industrial Crystallization (Dr. IYVLT, Research Institute of Inorganic Chemistry, Revoluční 86, CS-400 60 Ustí nad Labem, Czechoslovakia)	Ustí nad Labem (Czechoslovakia)
September 1–5	EUCHEM Conference on Useful Preparative Aspects of Photochemistry (Dr. D. DE KEUKELEIRE, Laboratorium voor Organische Chemie, Rijksuniversiteit Gent, Krijgslaan 271. S.4, B-9000 Gent, Belgium)	Gent (Belgium)
September 1–5	II World Conference on Computers in Education (Mr. J. HEBENSTREIT, École Supérieure d'Électricité, 10 Avenue Pierre-Larousse, F-92240 Malakoff, France)	Marseille (France)
September 8–10	6th European Food Symposium (Dr. R. JOWITT, National College of Food Technology, St. George's Avenue, Weybridge, Surrey, UK)	Cambridge (UK)
September 9–12	II International Symposium on Tests on Bitumins and Bituminous Materials (Symposium Secretariat, Hungarian Chemical Society, Anker Kőz 1, H-1061 Budapest, Hungary)	Budapest (Hungary)

September 15-19	4th European Symposium on Corrosion Inhibitors (Secretariat, 4 SEIC, Istituto Chimico, University of Ferrara, Via Scandiana 25, I-44100 Ferrara, Italy)	Ferrara (Italy)
September 17-19	Conference on Polymer Rheology and Plastics Processing (Plastics Institute, 11 Hobart Place, London SW1W 0HL, UK)	Loughborough (UK)
September 21-26	26th Meeting of International Society of Electrochemistry: Electrochemistry in Nonaqueous Solutions (26th ISE Organizing Committee, Verein Österreichischer Chemiker, Eschenbachgasse 9, A-1010 Wien, Austria)	Baden bei Wein (Austria)
September	Symposium on Transplutonium Elements and Plutonium Ceramic Materials (Prof. W. MÜLLER, European Institute of Transuranium Elements, Kernforschungszentrum Karlsruhe, Postfach 22600, D-7500 Karlsruhe, Federal Republic of Germany)	Baden-Baden (Federal Republic of Germany)
October 7-11	4th International Nuclear Industries Fair and Technical Meetings (Secretariat NUCLEX 75, Swiss Industries Fair, CH-4000 Basel 21, Switzerland)	Basel (Switzerland)
November 10-11	International Symposium on Energy Saving in Chemical Processes (FAST, Piazzale R. Morandi 2, I-20121 Milan, Italy)	Milan (Italy)
November 30 -December 5	I North American Chemistry Congress (Secretario Científico del Congreso, Sociedad Química de México, Apartado Postal 4-875, Ciprés 176, México 4, DF, México)	México City (México)
December 3-9	VI International Congress on Metallic Corrosion (Conference Secretary, VI International Congress on Metallic Corrosion, POB 391, Darlinghurst, New South Wales, Australia 2010)	Sydney (Australia)

International Union of Pure and Applied Chemistry

COMPTES RENDUS XXVII CONFERENCE

MUNICH, 21 – 31 AUGUST 1973

The biennial Conference of the International Union of Pure and Applied Chemistry (IUPAC) provides the occasion for its Council to assemble. Delegations from the 44 member countries make it a truly international gathering.

Council, being responsible for the policy of the Union, receives reports on all major activities undertaken in the name of IUPAC. These reports and the deliberations of Council are recorded in Part B of the COMPTES RENDUS. In particular, the "President's Report on the State of the Union" constitutes an excellent summary of progress achieved, at the international level, towards solving those problems of mankind in which the discipline of chemistry figures in a major or minor role.

In addition to Council, several standing committees (Clinical Chemistry, Machine Documentation, etc.) and some 30 specialist committees attached to the six IUPAC Divisions (Physical, Inorganic, Organic, Macromolecular, Analytical, and Applied Chemistry) met in Munich. The reports of their meetings in Part B of the COMPTES RENDUS cover the many topics of international importance to pure and applied chemistry currently under study for regulation, standardization or codification by the Union.

Part A of the COMPTES RENDUS comprises a comprehensive listing of all IUPAC committees, including the names and addresses of the more than six hundred members who belong to them.

This invaluable reference work is available only from the IUPAC Secretariat.

1974 Part A, 126 pp; Part B, 342 pp £3.00 (US \$9.00)

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The International Union of Pure and Applied Chemistry has published the journal **PURE AND APPLIED CHEMISTRY** in conjunction with Butterworths, for over ten years, so that chemists everywhere could benefit from the large amount of very important material handled each year by the Union. It was felt that matters of international importance had often not received a sufficiently wide circulation to make them easily available throughout the world. The journal has two objects: firstly to publish the main invited lectures of symposia sponsored by **IUPAC**, and secondly to publish the recommendations of the Union's Commissions on nomenclature, symbols and such matters as standard analytical procedure.

It is proposed to publish four volumes in 1975 of **PURE AND APPLIED CHEMISTRY**, each volume containing approximately 600 pages. Should the Union consider additional material is of sufficient importance this will be issued as a bound volume supplementary to the journal.

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1974. 1318 pages. \$90.00 (£30.00) ISBN 0 408 70566 3

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1. General Introduction.
2. Reference Materials for Thermometric Fixed Points.
3. Temperature Measurement under Pressure.
4. (Part 1). Pressure Measurements 1—Mercury Absolute Manometers. (Part 2). Pressure Measurements II—Pressure Scale and Fixed Point. (Part 3). Pressure Measurements III—Piston Gages. (Part 4). Pressure Measurements IV—Secondary Gage-Differential Manometers. (Part 5). Pressure Measurements V—Instruments for Relative Pressure Measurements. (Part 6). Pressure Measurements VI—Pressure Measurements for the Range 1 kPa to 100 uPa. (Part 7). Pressure Measurements VII—Very Low Pressures and Ultra Low Pressures (below 10^{-6} Torr).
5. The Absolute Measurement of Volume.
6. Measurement of p-V-T Properties of Gases and Gas Mixtures at Low Pressure.
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8. p-V-T Relationships in Gases at High Pressure and High Temperatures.
9. The Compression of Liquids.
10. Determination of Thermodynamic Properties from the Experimental p-V-T Relationships.
11. Thermodynamic Properties and the Velocity of Sound.
12. Relation of the Dielectric Constant and the Refractive Index to Thermodynamic Properties.
13. Vapor Pressures.
14. Thermodynamic Properties near the Critical State.
15. Solubility.
16. (Part 1). Phase Equilibria (General Procedure) 1—Phase Equilibria of Two-component Systems and Multicomponent Systems. (Part 2) Phase Equilibria (General Procedure) II—Phase Equilibria of Liquid and Gaseous Mixtures at High Pressures.
17. (Part 1). Liquid-Solid Phase Equilibria 1—Melting Points and Volume Changes. (Part 2). Liquid-Solid Phase Equilibria II—Cryoscopy.
18. EMF Measurement in Molten Salts.
19. (Part 1). Thermodynamic Properties of Fluid Metals I—Medium and Low Pressures. (Part 2). Thermodynamic Properties of Fluid Metals II—High Temperatures and High Pressures.
20. Interphase Surface Tension.
21. Adsorption.
22. Chemical Relaxation in Liquid Systems.
23. Thermodynamic Properties from Shock Waves.
24. Electrical Discharge Techniques for Measurements of Thermodynamic Properties of Fluids at High Temperatures.
25. The Ballistic Compression and High Temperature Properties of Dense Gases.
26. Thermodynamic Properties of Fluids below 20 K.

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International Union of Pure and Applied Chemistry

CRITICAL EVALUATION OF SOME EQUILIBRIUM CONSTANTS INVOLVING ORGANOPHOSPHORUS EXTRACTANTS

Edited by Y. MARCUS

CONTENTS

Introduction

- I $H^+ + DBP^- = HDBP$
- II $HDBP = \overline{HDBP}$
- III $2 \overline{HDBP} = \overline{(HDBP)_2}$
- IV $1/2 \overline{(HDBP)_2} + \overline{TBP} = \overline{HDBP \cdot TBP}$ and
 $\overline{(HDBP)_2} + \overline{TBP} = \overline{(HDBP)_2 \cdot TBP}$
- V $TBP = \overline{TBP}$
- VI $H_2O + \overline{TBP} = \overline{H_2O \cdot TBP}$
- VII $H^+ + NO_3^- + \overline{TBP} = \overline{HNO_3 \cdot TBP}$
- VIII $H^+ + Cl^- + \overline{TBP} = \overline{HCl \cdot TBP}$
- IX $H^+ + DE-HP^- = HDE-HP$; $HDE-HP = \overline{HDE-HP}$;
 $2 \overline{HDE-HP} = \overline{(HDE-HP)_2}$
- X $1/2 \overline{(HDE-HP)_2} + \overline{TBP}$ (or $\overline{TO'PO}$) = $\overline{HDE-HP \cdot TBP}$
(or $\overline{TO'PO}$); $\overline{(HDE-HP)_2} + \overline{TBP}$ (or $\overline{TO'PO}$) =
 $\overline{(HDE-HP)_2 \cdot TBP}$ (or $\overline{TO'PO}$)
- XI $UO_2^{2+} + 2NO_3^- + 2\overline{TBP} = \overline{UO_2(NO_3)_2(TBP)_2}$
- XII $Pu^{4+} + 4NO_3^- + 2\overline{TBP} = \overline{Pu(NO_3)_4(TBP)_2}$
- XIII $H^+ + NO_3^- + \overline{TO'PO} = \overline{HNO_3 \cdot TO'PO}$
- XIV $UO_2^{2+} + 2NO_3^- + 2\overline{TB'PO} = \overline{UO_2(NO_3)_2(TB'PO)_2}$
- XV $H^+ + NO_3^- + \overline{DBB'P} = \overline{HNO_3 \cdot TBB'P}$
- XVI $UO_2^{2+} + 2NO_3^- + 2\overline{DBB'P} = \overline{UO_2(NO_3)_2(DBB'P)_2}$

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LIST OF ABBREVIATIONS

ACS	American Chemical Society
AFNOR	Association Francaise de Normalisation
AOAC	Association of Official Analytical Chemists
AOCS	American Oil Chemists Society
CBN	IUPAC-IUB Commission on Biochemical Nomenclature
CEBJ	IUB Commission of Editors of Biochemical Journals
CEE	Communauté Européenne Economique
CIC	Chemical Institute of Canada
CID	Comité Internatioanl des Dérivés Tensio-Actifs
CMN	IUPAC Commission on Macromolecular Nomenclature
CNIC	IUPAC Commission on Nomenclature of Inorganic Chemistry
CNOC	IUPAC Commission on Nomenclature of Organic Chemistry
CNRS	Centre National de la Recherche Scientifique in France
CQUCC	IUPAC Commission on Quantities and Units in Clinical Chemistry
DIN	Deutsche Industrie-Norm
EFEMA	European Food Emulsifier Manufacturers Association
EP on EQ	Expert Panel on Quantities and Units of IFCC Committee on Standards
FAO	UN Food and Agriculture Organization
FATIPEC	Fédération d'Associations de Techniciens des Industries des Peinture
FECs	Federation of European Chemical Societies
FIP	Fédération Internationale Pharmaceutique
FSPT	US Federation of Societies of Paint Technology
IAEA	International Atomic Energy Agency
IARC	WHO International Agency for Research on Cancer
IASC	International Association of Seed Crushers
ICC	International Association for Cereal Chemistry
ICCCI	International Coordinating Committee of the Coatings Industry
ICSU	International Council of Scientific Unions
ICSU AB	ICSU Abstracting Board
IDCMD	IUPAC Interdivisional Committee on Machine Documentation
IFCC	International Federation of Clinical Chemistry
ISE	International Society of Electrochemistry
ISO	International Organization for Standardization
ISO/TC	ISO Technical Committee
ISO/TC SC	ISO/TC Sub-Committee
IUB	International Union of Biochemistry
IUCr	International Union of Crystallography
IUFoST	International Union of Food Science and Technology
IUNS	International Union of Nutritional Sciences
IUPHAR	International Union of Pharmacology
IUPS	International Union of Physiological Sciences
NATO	North Atlantic Treaty Organization
NBS	US National Bureau of Standards
NSF	US National Science Foundation
OICC	Office International du Cacao et du Chocolat
PAG	Protein Advisory Group of FAO/WHO/UNICEF
SLF	Federation of Scandinavian Paint and Varnish Technicians
UN	United Nations
UNESCO	UN Educational, Scientific, and Cultural Organization
UNICEF	UN Children's Fund
WHO	UN World Health Organization
WPSPF	Working Party on Supported Polymer Films of IUPAC Macromolecular Division

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**INTERNATIONAL UNION OF PURE
AND APPLIED CHEMISTRY**

**INFORMATION BULLETIN
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NOVEMBER 1975

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International Union of Pure and Applied Chemistry
1975

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Treasurer	— Prof. O. HORN (Federal Republic of Germany)

IUPAC INFORMATION BULLETIN

The Bulletin provides a news medium for the various activities of IUPAC, especially of its 50 or so committees which deal with chemical topics needing regulation, standardization or codification. It carries advance information on forthcoming symposia which are to be sponsored by IUPAC together with reports of such meetings which have recently taken place. Coverage is also given to projects in which IUPAC is collaborating with other international organizations.

Two series of Appendices to the Bulletin are issued:

- (i) Appendices on Provisional Nomenclature, Symbols, Units, and Standards
- (ii) Technical Reports

The publishing arrangements and subscription rates for the Bulletin in 1976 are under review (see p. 3). Details will be announced shortly.

To all our Readers

Extracts from the *Information Bulletin* may be reproduced freely in university bulletins, industrial house magazines, information newsheets, and national journals. In particular, IUPAC will be pleased for attention to be drawn to the availability of its new publications and to the dates and subjects of forthcoming international symposia of the Union.

International Union of Pure and Applied Chemistry

Recommended Reference Materials for the Realization of Physicochemical Properties

There are many measuring systems and instruments in use today which yield results whose uncertainty of measurement and limits of error cannot be established without the employment of materials with known properties. Materials used for this purpose are called reference materials. In 1972 the IUPAC Commission on Physicochemical Measurements and Standards published a "Catalogue of Physicochemical Standard Substances" in **Pure and Applied Chemistry** (Vol. 29, No. 4, pp. 597 - 616).

However, it was realized that a more comprehensive compilation was needed and a Sub-Commission on Calibration and Test Materials was set up to prepare recommendations on the selection and specification of reference materials for use in various types of physicochemical measurement. The first batch of the Sub-Commission's recommendations have now been issued in sections dealing with General Introduction (to the whole series), Enthalpy, Optical Rotation, and Surface Tension. Further sections will be published as more recommendations become available.

Published in **Pure and Applied Chemistry** Vol. 40, No. 3 (1974) and available as a reprint (approx. 84 pages), price £2.00 (US-\$6.00) surface post or £2.66 (US-\$8.00) airmail from IUPAC Secretariat, Bank Court Chambers, 2-3 Pound Way, Cowley Centre, Oxford OX4 3YF.

IUPAC publications are available in the USA and Canada from Crane, Russack & Co., 52 Vanderbilt Avenue, New York, NY 10017.



Dr. R.W. Cairns (USA)

1975-77

28th IUPAC CONFERENCE

Madrid: 2-11 September 1975

At the conclusion of the above Conference, the Presidency of the Union was assumed by Dr. R. W. CAIRNS (USA).

Curriculum Vitae of New President

ROBERT W. CAIRNS, Executive Director of the American Chemical Society, was born on 23 December 1909, in Oberlin, Ohio. He was educated at Oberlin College (A.B., 1930) and Johns Hopkins University (Ph.D. in Chemistry, 1932). He participated in the Advanced Management Program of Harvard Business School in 1951, and holds an honorary degree of Doctor of Science awarded by the University of Delaware in 1969.

Dr. CAIRNS began his distinguished career in pure and applied chemistry in 1934 as a research chemist at the Research Center of Hercules Inc., where he worked on high explosives and propellants, cellulose, resin, and terpene chemistry, polymer chemistry, and petrochemicals. He became Director of the Research Center in 1941, Director of Research for Hercules Inc. in 1955, member of the Board of Directors in 1960, and Vice-President, Research in 1965. In 1971, following his retirement from Hercules, he was appointed Deputy Assistant Secretary for Science and Technology in the US Department of Commerce. In 1972, he accepted his present position as chief staff officer of the American Chemical Society.

Culminating long service to the US Department of Defense as a consultant, Dr. CAIRNS served as Deputy Assistant Secretary of Defense during 1953-1954 and has served two terms as a member of the Defense Science Board.

Dr. CAIRNS is an honorary member of the Société de Chimie Industrielle. He received the Perkin Medal awarded by the American Section of the Society of Chemical Industry in 1969. He was elected to the National Academy of Engineering in 1969 and has been a member of the Executive Committee of the Academy's Council. He was chairman of a major study of scientific and technical communication jointly sponsored by the National Academy of Engineering and the National Academy of Sciences in 1966-1970. He is a past President of the American Chemical Society, and has been a member and chairman of the Board of Directors. He was Science Advisor to the Governor of Delaware from 1969 to 1971, and has served also as a member of the Panel on Government Laboratories of the President's Science Advisory Committee. He has been a Director of the Industrial Research Institute and is a past President of the Institute, and received the IRI Medal for 1974.

Dr. CAIRNS is a past chairman of the National Research Council's Division of Chemistry and Chemical Technology. He has long been actively interested in IUPAC, was an appointed member of the US National Committee for IUPAC from 1958 to 1964 and served as a Council delegate from USA in 1961, 1963, 1965, 1969, and 1971. In 1967 he was elected a member of the Applied Chemistry Division Committee, became Vice-President of the Division in 1969, and President in 1971. He was elected Vice-President (President-Elect) of IUPAC in 1973.

Other Officers

As a result of the elections held at the Council meeting on 11 September, the other Officers of the Union are:

Vice-President (President-Elect 1977)

Prof. G. SMETS (Belgium)

Secretary General (1975-9)

Prof. G. OURISSON (France)

Treasurer (1971-9)

*Prof. O. HORN (Federal Republic of Germany)

Bureau

During the interval between the biennial meetings of Council, the Bureau is responsible for ensuring an orderly discharge of the functions of the Union.

In addition to the Officers of the Union, the following are now automatically Members of the Bureau:

Past-President (1975-7)

Prof. Sir HAROLD THOMPSON (UK)

Division and Section Presidents

Dr. R. N. JONES (Physical Chemistry Division: 1973-7)

Prof. L. MALATESTA (Inorganic Chemistry Division: 1975-7)

Prof. H. ZOLLINGER (Organic Chemistry Division: 1975-7)

Prof. C. G. OVERBERGER (Macromolecular Division: 1975-7)

Prof. N. TANAKA (Analytical Chemistry Division: 1973-7)

Dr. H. EGAN (Applied Chemistry Division: 1973-7)

Prof. P. LOUS (Clinical Chemistry Section: 1975-7)

The 12 Elected Members of the Bureau are now:

Prof. A. ABOU-EL-AZM (Arab Republic of Egypt: 1975-9)

Prof. Sir DEREK BARTON (UK: 1973-7)

Prof. A. R. H. COLE (Australia: 1973-7)

Dr. M. A. CRIVELLI (Argentina: 1975-9)

*Prof. N. M. EMANUEL (USSR: 1971-9)

Prof. O. GLEMSER (Federal Republic of Germany: 1973-7)

Prof. V. HEROUT (Czechoslovakia: 1969-77)

*Dr. O. ISLER (Switzerland: 1971-9)

Prof. S. NAGAKURA (Japan: 1975-9)

Prof. A. PEREZ-MASIÁ (Spain: 1975-9)

Prof. S. RANGASWAMI (India: 1969-77)

Prof. H. SUOMALAINEN (Finland: 1969-77)

New Associated Organizations

Council approved applications for Associated Organization status from the following international organizations whose aims and activities are in harmony with those of IUPAC:

Association of Editors of European Chemistry Journals

Groupe pour l'Avancement des Méthodes Spectroscopiques et Physico-Chimiques d'Analyse

International Association for Water Pollution Research

International Committee on the Science of Photography

International Confederation for Thermal Analysis

International Organization for Crystal Growth

*Reelected at Madrid for a further period of 4 years.

Publications

In 1958 the Union appointed Butterworths as its official publisher, since when the work of IUPAC has been brought together successfully in *Pure and Applied Chemistry**, the *Information Bulletin* with its Appendices, the sets of Nomenclature Rules, the *Comptes Rendus*, and in other separate issues. During the last 2 years, however, there have been unjustifiable delays by the publisher and perhaps inadequate advertising and sales service. After inviting applications from a number of publishing companies in different countries, the Union has decided to terminate its present contract and that Pergamon Press should take over the work at the end of 1975. It is expected that Pergamon will also assume responsibility for printing and distributing the *Information Bulletin*, and details of the subscription rates for the Bulletin in 1976 will be announced shortly.

Reclamation of Solid Wastes

After considering reports from an *ad hoc* Committee, IUPAC approved the establishment of a Commission on Solid Wastes attached to the Applied Chemistry Division. The Commission will identify problems with the collection, processing, and reclamation of solid wastes, and stimulate the appropriate governments and bodies to support key research on these problems.

1977 IUPAC Conference

Council accepted an invitation from the Polish National Committee for Chemistry of the Polish Academy of Sciences to hold the 29th IUPAC Conference (1977) in Poland. The exact location is still under consideration, but the probable dates are during the last week of August. This will enable participants to travel subsequently to Tokyo for the 26th IUPAC Congress on 4-10 September 1977 (see p. 157). Also it was decided to hold the 30th IUPAC Conference (1979) in Switzerland, and that the 27th IUPAC Congress (1979) should provisionally be in Finland.

A revised version of the IUPAC Statutes and Bylaws (1965) was approved by Council in Madrid. One consequence is that the IUPAC biennial *Conference* will henceforth be known as the *General Assembly*. It is hoped that this change will more readily indicate the difference between the *Conference* and the *Congress* of the Union.

Comptes Rendus 28th IUPAC Conference

The full deliberations of Council, together with reports of meetings of nearly 50 Standing Committees, Division Committees, Sections, Commissions, and Sub-Commissions, held during the Conference in Madrid, will be published as *Comptes Rendus 28th Conference* (details to be announced later). The *Comptes Rendus* will also contain the new memberships of all IUPAC bodies.

*Please note that all subscription renewals for 1976 should be sent to the Journals Subscription Department, Pergamon Press Ltd., Headington Hill Hall, Oxford OX3 0BW, UK, instead of to Butterworths.

CHEMISTRY IN A CHANGING WORLD— A LOOK AHEAD*

The work of cosmologists, geologists, and archaeologists indicates that the planet earth has been in existence for about six billion years and that primitive man may have made his first appearance upon it something like two million years ago. While accepting these estimates, it is however true that, for all practical purposes, the world as you and I know it today is not much more than a century and certainly less than two centuries old. If I was asked to be more precise, I would say about a century and a quarter—since somewhere around 1850. Some would date it from the invention of the steam engine towards the end of the eighteenth century, which, they would claim by placing in man's hands almost unlimited but controllable mechanical power and so triggering off the Industrial Revolution, really marked the beginning of the modern world. In a sense this is true, for the great upsurge of industrial activity together with the growth in population and the increase in wealth and leisure resulting from that revolution were major factors in the development of science during the nineteenth century. Yet the industrial revolution itself was in principle little different from earlier technological advances during mankind's history—it was, like all the others from agriculture onwards, based on the exploitation of chance discovery or invention. What ushered in the new world—that in which we live—was the conscious application of science to the solution of practical problems and this I submit really began about the middle of last century.

Why it should have occurred at that particular juncture is something which could form the subject of an extended and complex debate upon which I do not wish to embark in this lecture. I can, however, give in very brief outline my own picture of the situation. As I have already indicated, I believe that the industrial revolution was new in man's history only in the scale of the effects produced by the exploitation of the inventions on which it rested and notably by the steam engine. But the great increase in wealth resulting from it and the bustling, thrusting character which it evoked in society, had a profound influence on a wide variety of human pursuits including science. After many centuries during which it made little progress, natural science really began to develop as a result of the so-called scientific revolution in the latter half of the seventeenth century, when the experimental method was adopted as the only true approach to the investigation of the natural world. From that time onwards its development, although steady, was comparatively slow and, moreover, since it remained very largely in the hands of amateurs, it had little influence on everyday life and affairs. It burgeoned, however, like so much else during the Industrial Revolution and somewhere around the middle of the nineteenth century men began to apply its methods to the problems of industry, agriculture, and medicine. The success of the early pioneers—W. H. PERKIN, the discoverer of mauveine and father of the synthetic dyestuff industry is a good example—was such that everything snowballed. New industries arose and with the chance element in discovery being in substantial measure reduced, the rate of technological advance increased continuously not only during the rest of the nineteenth but at a still accelerating pace during the twentieth century up to the present day. Yet quite suddenly, after all our technological successes, a feeling of doubt and uncertainty has made its

*A lecture presented on 10 September in Madrid by Lord TODD (UK), a former President of the Union, to participants at the 28th IUPAC Conference.

appearance—a feeling made even stronger by the worldwide economic effects of the oil crisis. People throughout the world are today worried in varying degree about energy, about population, about food, and about pollution and the deterioration of our natural environment. There is no need to accept the views of those sometimes referred to as ‘doomwatchers’ in order to appreciate that we seem to be again at a turning point in the advance of civilization and that this is a very good time to look at our world and to consider its future.

That we in the International Union of Pure and Applied Chemistry should do so is peculiarly appropriate for there is in my mind no doubt that the utter dependence of our material civilization upon chemistry and the technologies deriving from it makes our science the central feature of the modern world and the hope of its future. I do not claim that other sciences are unimportant, but I do claim that the great discoveries in, for example, physics and biology, would for the most part have remained scientific curiosities without the assistance of chemistry which has provided that materials which alone made them practically useful. We are indeed the bridge between science and technology in many areas of endeavour.

Now wherein does the world of today differ from that of the pre-Industrial Revolution era? I would say that the most striking differences are in population, in agriculture, in medicine, in energy utilization, in communication, and in substitution of traditional materials of natural origin by new and more flexible products stemming from the chemical industry. Of course, the magnitude of the difference varies from one part of the world to another; therein indeed lies one of our major problems today for the disparity in living standards between the highly industrialised countries in the world and the underdeveloped or developing areas is a source of dangerous social and political instability. World population is still rising at an alarming rate. Already at nearly four billion, more than twice what it was in 1900, it will have reached six billion by the end of this century and unless some measures are taken soon it will have doubled again in another forty or fifty years from then. This rise in population is probably unconnected with any increase in fertility. It stems rather from the increase in material wealth consequent on the industrial revolution, from the enormous expansion and development of food production through agriculture, and on improved sanitation and public health. More recently it has also been quickening through medical advances, *e.g.*, the lowering of infant mortality and the control of infectious disease.

For all of these the chemist must accept a major share of responsibility. The growth in food production necessary to meet the needs of a rapidly rising population doubtless owed something to changes in land tenure and the scale of agricultural operations, but the major factor was surely the introduction and development of artificial fertilizers and more recently the control of weeds and other agricultural pests by the agrochemical industry. Without these the new high yielding strains of food plants produced by the plant breeders would have been of little value if indeed they would have been produced at all. Public health and sanitation also rest heavily on chemistry to provide materials needed for treatment of sewage, industrial effluents and other pollutants, a need which has not diminished with the passage of time and today looms as large as ever. Medical advances have drastically lowered infant mortality and so reduced the menace of infective disease as well as many other organic ailments, that life expectancy has been greatly lengthened. Through this a radical change in the age structure of our population is now

taking place with consequences which have not as yet been fully appreciated. It is from chemistry, or rather from its application in the pharmaceutical industry, that most of this development has come. It is indeed no exaggeration to say that there has hardly been an advance in therapy during the past fifty years which has not originated in the pharmaceutical industry rather than in medicine itself, while a goodly part of surgical progress must be ascribed to the availability of improved anaesthetics, muscle relaxants, and so on.

Almost hand in hand with these advances in agriculture and medicine have come vast improvements in the comfort and quality of life, especially in the so-called advanced countries. For one thing communications have been enormously improved—life would be very different without the aeroplane, telephone, radio, television, and all the multitude of electrical and electronic marvels which we take for granted. But let us not forget that these rest for their successful use on new materials for insulation, on semiconductors, and on many another material provided by the chemist. Moreover, it is to chemistry that we owe the new materials which have replaced and for particular uses improved upon so many products of natural origin. Among these we can think of the enormous range of plastic and polymeric materials substituting for wood, rubber, and in some cases metal; artificial fibres; packaging materials; elastomers; and detergents. These are but a few examples of the multitude of products of the chemical industry which we nowadays take for granted as part of the normal fabric of our daily life.

Developments such as those I have mentioned have only been made possible by enormously increasing the demands made on our energy sources—mainly so far on the so-called fossil fuels—coal, oil, and natural gas—with subsidiary usages of water and geothermal power. Wind and tidal power, like solar energy, have been as yet little exploited. The latest newcomer to the field is of course nuclear energy, as yet developed only on a modest scale but undoubtedly an energy source of enormous importance to our future. The development of nuclear energy has imposed major demands on chemistry, not merely for fuel elements, but also for new coolants, materials of construction, and so on. Even the development of power units based on more traditional fuels, such as gas turbines and jet engines, has required new alloys and other new materials of construction. Wherever one looks—there is chemistry.

The importance of chemistry in the development of the world as we know it today is therefore in my view at least, beyond dispute. However, the question many people ask is whether the result achieved by all this activity would not suggest a much less important role for it in the future. In recent years there has been a sudden and at times over-emotional reaction to the problems of our day—problems which in some cases have arisen because we have in the past given no thought to the longer term consequences of our actions. To put the matter very simply, people point to the over-population and frequent famines characteristic of a number of areas in the world today and query how long world food supply can match our growing population. They further point to our prodigal use of nonrenewable natural resources such as minerals, to our ever-increasing inroads upon our necessarily limited reserves of fossil fuels, and to the growing hazards of pollution from industrial effluents, sewage, power plants involving nuclear fission, and excessive use of organic and artificial fertilizers leading to pollution of rivers and streams with, for example, nitrates.

Now, all these dangers are real and although one can perhaps dismiss some of the more alarmist predictions that are made, we must all of us recognize

that they must be faced and solutions to them found in the near future if a catastrophic situation for mankind is to be avoided. Some there are who cry 'Away with science; it has got us into this mess so get rid of it and return to the good old days before it took charge'. This is, of course, an idle dream. We cannot go back even if we would and in any case it is more than doubtful whether there ever were any 'good old days' to look back on; life is now infinitely easier and more pleasant than it was for our forebears a couple of centuries ago. There is, in fact, no way out of our difficulties save through science and the technology based upon it. And just as chemistry has been a prime factor in our development for the past century and more, so it will be in the future.

In looking ahead, be it in chemistry or indeed any other activity, we must begin by making one assumption, namely, that human population will be brought under control within a reasonably short time. I do not underrate the difficulty of doing so by deliberate action, but I am convinced that the difficulty must be faced and conquered. Otherwise control will come through biological response which will be much slower and more painful and could well be accompanied not just by falling living standards but by an actual physical and mental deterioration of the species. Population apart, man's primary problem is energy. Energy dominates not just the paraphernalia of industrial civilization, but the whole of biology or, if you like, of life on this or, indeed, any other planet. Because it is fundamental to the chemical industry in more ways than one, I must begin by making a few comments about it.

The most convenient and so the most widely used sources of energy for industry are the fossil fuels—natural gas, petroleum, and coal in various forms. There are substantial reserves of these and doubtless more will be discovered—the seabed, for example, remains largely unexplored. Nevertheless, our resources are finite and are being used up much more rapidly than they are being generated. The fossil fuels can be described as hydrocarbon sources and energy is produced by oxidizing these to carbon dioxide. But, because of its flexibility, carbon is central to most of modern chemical industry and by far the most convenient source of carbon for this purpose is petroleum (and to a lesser extent I suppose, natural gas). It would surely be common prudence to conserve the major part of our petroleum for this purpose and use the less chemically convenient coals for energy production. To some extent, but not I think sufficiently, this has already been recognized and the proportion of petrochemical feedstock (naphtha) produced by the petroleum refiners has been increasing in recent years; unfortunately, of course, naphtha is in competition with gasoline which comes from the same oil fraction. This is likely to remain a very serious problem unless and until thermonuclear power becomes a realistic possibility—a thing which I think will not be achieved until next century. Nuclear power by fission processes is never likely to provide more than a small part of our energy requirements; apart from anything else the radioactive waste problem will impose limits to its use. With unlimited low-cost thermonuclear power, petroleum could be reserved for chemical use. But even if petroleum was no longer available it would be possible to use carbon dioxide rather than hydrocarbons as the raw material for the chemical industry.

Hitherto for reasons of ease, convenience, and cost, we have based much of our industry on hydrocarbons; these we have used to build up other materials and also to provide energy by oxidizing them to carbon dioxide. We should, however, remember that there is no *a priori* reason why, given another unlimited source of energy, we should not reverse the process and, using

carbon dioxide as our raw material, make from it hydrocarbons and indeed all the other products of the organic chemical industry. After all, this is precisely what the vegetable world is doing every day on a gigantic scale. Plants, of course, use the sun as their energy source for this purpose. No doubt we both could and will make in the future much more use of solar energy than we now do, but owing to the intervention of night and day and the incidence of variable cloud cover over the earth, solar energy is rather a tricky source to handle. I believe that in the longer term it will be more attractive to use controlled nuclear fusion as our energy source—it is, of course, the source used by the sun but it might well be harnessed by us. So much at least is suggested by recent experimental work on plasma containment.

I have already drawn attention to the fact that, whether we like it or not, that can be no stabilization of world population before our numbers are roughly double what they now are—short, that is, of some cataclysmic natural disaster. These huge numbers will have to be fed and hence there will have to be great emphasis on food production and especially on agriculture. It follows that there will be continued growth in such branches as the fertilizer and agrochemical industries, the former to stimulate the growth of crops and the latter to control plant and animal pests both in growing crops and in stored food products. As regards fertilizers, the primary need is and will remain the provision of the elements nitrogen, phosphorus, and potassium in forms available to the growing plant. We have, I suppose, all become accustomed to a more or less static picture of ammonia, nitrate, phosphate, and potassium salts together with urea which, although not agronomically ideal, does provide a relatively concentrated nitrogen source. It would, I think, be fair to say that present fertilizers are very wasteful as regards phosphate and nitrate in particular and new materials offering slow release of important ions and avoidance of pollution by runoff are necessary. I believe that the industry will indeed produce such new materials. As regards phosphate, it might be possible to use quite novel types of phosphorus compound based on the element itself rather than, as now, phosphoric acid. Again, organic derivatives of nitrogen such as oxamide may assume increasing importance. I do not think that cost need prevent such developments because the new fertilizers will be needed in much smaller quantity than the present types.

The fertilizer situation could, of course, be greatly affected if some of the work now in progress on the fixation of atmospheric nitrogen by chemical and biological means had a successful outcome. It has already been shown that nitrogen fixation by purely chemical means using organometallic compounds (e.g., of molybdenum and titanium) is possible. Although it is difficult to see any commercial future for the use of these particular materials, further research may lead in time to better variants. On the biological side much interest attaches to the incorporation or integration of nitrogen-fixing bacterial systems with important food crops. The degree to which this approach can succeed remains to be seen, but even if it does not one cannot rule out the possible isolation, immobilization, and subsequent use on the large scale of the bacterial enzymes responsible for fixing atmospheric nitrogen.

The emphasis on agriculture must also involve increasing emphasis on pest control as crop yields are forced up. Although biological control methods will doubtless increase, I believe that the main burden will continue to be carried by the agrochemical industry where I expect to see the development of products with higher specificity in action coupled with greater sophistication in use.

What I foresee in the fertilizer and agrochemical industries does, in fact, typify the trends I expect to see followed in the chemical industry as a whole. They might well be summed up by the phrase 'increasing sophistication'. There will be new materials but these will not, in the main, be radically new types but rather precisely tailored products to meet specialized needs and, even more, there will be new approaches to economical energy-sparing and especially pollution-avoiding processes of production. On the new material side I expect to see a considerable expansion in the field of inorganic chemistry. This will involve not only inorganic polymers, but compounds of carbon with many other elements. There remains a great deal of undeveloped potential in such materials as silicon nitride, carbon fibres, and so on. But it seems to me that it is in the development of new types of process for the production of existing as well as of new materials that the biggest changes may come. This is a prediction I make with considerable confidence because the beginnings of such developments are already visible.

Microorganisms have long played a vital part in, for example, brewing, tanning, and the food industries, but until the discovery of the antibiotics they were hardly used elsewhere. The revelation of the astounding synthetic ability of microorganisms as antibiotic producers led in due course to their successful application in the field of medicinal chemistry, *e.g.*, in the hydroxylation of steroids. In recent years very important advances have been made, firstly through the isolation, purification, and stabilization of the enzyme systems in microorganisms responsible for particular reactions and especially in the so-called immobilization of these enzymes by attachment to support materials of various types. These so-called 'immobilized enzymes' are potentially of the greatest importance and are even now being intensively studied for large scale application in industry. The most immediately obvious uses of such enzymes would be in such processes as the saccharification of cellulose and it could well be that some such processes may soon be in operation. Related in some respects to the immobilized enzyme approach is the use of polymer supports in the conduct of polycondensation procedures, *e.g.*, the Merrifield method for polypeptide synthesis. It may still be a long way from practical large scale application, but when one reflects on the extraordinary ease and efficiency with which proteins are synthesized by living cells on a nucleic acid template by just such methods, it would be rash to deny their industrial possibilities.

In this lecture I have tried in a very general way to look at chemistry and the industries based upon it in the light of the rapidly changing circumstances of our time. There are, I know, many who feel that the change is an accelerating deterioration of the world from mankind's viewpoint and who predict early and total disaster. I do not share this view—or, perhaps better expressed—I do not believe disaster need come if we use the immense resources of our science and technology. And among these resources those of chemistry stand high in importance. I believe in our subject and in the potential of our industry. Our efforts can contribute to a new and better future for all of us. So let us bend our efforts to that end—but let us do so quickly for the need is urgent and time is not on our side.

IUPAC PUBLICATIONS

1974

A compilation of IUPAC Publications in 1973 was published in *Information Bulletin* No. 47 (March 1974). The present listing attempts to cover everything issued during 1974.

The IUPAC Secretariat would be pleased to receive notifications of any omissions from this listing, especially of translations completed or in process of being prepared of IUPAC nomenclature recommendations.

Pure and Applied Chemistry*

- Vol. 37, Nos. 1-2: Specially Invited Lectures from XI European Congress on Molecular Spectroscopy, Tallinn (USSR), May-June 1973
Commission on Radioanalytical Chemistry and Nuclear Materials: High Energy Photon Activation
Commission on Nomenclature of Organic Chemistry and IUPAC-IUB
Commission on Biochemical Nomenclature: Nomenclature of Cyclitols
- Vol. 37, No. 3: Main Section Lectures from two Joint Symposia held during XXIV IUPAC Congress, Hamburg (FRG), September 1973. Symposium on Medicinal Chemistry—Polypeptide Hormones and Releasing Factors. Symposium on Modern Methods for Treatment of Waste Water in Theory and Practice
- Vol. 37, No. 4: Commission on Analytical Nomenclature: Recommendations for Nomenclature of Thermal Analysis; Recommendations on Nomenclature for Chromatography; Recommendations on Nomenclature for Contamination Phenomena in Precipitation from Aqueous Solutions; Recommendations for Nomenclature of Mass Spectrometry
Commission on Microchemical Techniques and Trace Analysis: Trace Analysis Applicable to Determination of Minor Amounts of Impurities in Chemicals—I. General Survey
Commission on Electrochemistry: Electrochemical Nomenclature—being Appendix III to *Manual of Symbols and Terminology for Physicochemical Quantities and Units*
Commission on Quantities and Units in Clinical Chemistry and IFCC Committee on Standards, Expert Panel on Quantities and Units: Quantities and Units in Clinical Chemistry; List of Quantities in Clinical Chemistry
Commission on Electroanalytical Chemistry: An Approach to Conventional Scales of Ionic Activity for Standardization of Ion-selective Electrodes; *N*-Methylpropionamide as an Electrolytic Solvent—Purification and Properties
Commission on Atomic Weights: Atomic Weights of Elements 1973
- Vol. 38, Nos. 1-2: Specially Invited Lectures from XII and XIII Microsymposia on Macromolecules, Prague (Czechoslovakia), August 1973. XII Microsymposium: Organized Structures in Polymer Solutions and Gels. XIII Microsymposium: Transformations of Functional Groups on Polymers

*Official journal of IUPAC and additional publications of the Union are available from Butterworth & Co. (Publishers) Ltd., Borough Green, Sevenoaks, Kent TN15 8PH, UK. Much of the material which appears in the journal is made available shortly afterwards in book form for those persons who are interested only in purchasing specific material.

- Vol. 38, No. 3: Selected Plenary and Section Lectures from XV International Conference on Coordination Chemistry, Moscow (USSR), June 1973
IUPAC-IUB Commission on Biochemical Nomenclature: Nomenclature of Quinones with Isoprenoid Side-chains
- Vol. 38, No. 4: Plenary Lectures from III International Conference on Chemical Thermodynamics, Baden bei Wien (Austria), September 1973
- Vol. 39, Nos. 1-2: Specially Invited and Selected Symposium Lectures from International Symposium on Macromolecules, Aberdeen (UK), September 1973
- Vol. 39, No. 3: Specially Invited Lectures from International Symposium on Plasma Chemistry, Kiel (FRG), September 1973
- Vol. 39, No. 4: Plenary Lectures from II International Meeting on Boron Chemistry, Leeds (UK), March 1974
- Vol. 40, Nos. 1-2: Selected Specially Invited and Plenary Lectures from V International Symposium on Magnetic Resonance, Bombay (India), January 1974
- Vol. 40, No. 3: IUPAC-IUB Commission on Biochemical Nomenclature: Abbreviations and Symbols for Nucleic Acids, Polynucleotides and their Constituents: Abbreviations and Symbols for Description of Conformation of Polypeptide Chains; Nomenclature of Multiple Forms of Enzymes; Symbols for Amino-acid Derivatives and Peptides
Section on Air Quality: Analytical Methods for Use in Occupational Hygiene (Third Replacement-Addition Issue)
Sub-Commission on Calibration and Test Materials: Recommended Reference Materials for Realization of Physicochemical Properties
Commission on Macromolecular Nomenclature: List of Standard Abbreviations (Symbols) for Synthetic Polymers and Polymer Materials; Basic Definition of Terms Relating to Polymers
- Vol. 40, No. 4: Main Lectures from II International Conference on Physical Organic Chemistry, Noordwijkerhout (Netherlands), April-May 1974

Information Bulletin*

No. 47, March 1974

No. 48, October 1974

(Section on Fermentation: Recommendations on Education in Biochemical Engineering)

Appendices on Provisional Nomenclature, Symbols, Units and Standards

No. 34, August 1974: Proposed Terminology and Symbol for Transfer of Solutes from One Solvent to Another (Commission on Electroanalytical Chemistry)

No. 35, August 1974: Status of Faraday Constant as an Analytical Standard (Commission on Electroanalytical Chemistry)

No. 36, August 1974: Recommendations on Usage of the Terms 'Equivalent' and 'Normal' (Commission on Analytical Nomenclature)

No. 37, August 1974: Recommendations for Nomenclature and Spectral Presentation in Chemical Electron Spectroscopy Resulting from Excitation by Photons (Commission on Molecular Structure and Spectroscopy)

*Available from IUPAC Secretariat, Oxford.

- No. 38, August 1974: Recommendations for Presentation of NMR Data for Publication in Chemical Journals—B. Conventions Relating to Spectra from Other Nuclei (Commission on Molecular Structure and Spectroscopy)
 No. 39, August 1974: Definitions, Terminology, and Symbols in Colloid and Surface Chemistry—II. Heterogeneous Catalysis (Commission on Colloid and Surface Chemistry)
 No. 40, August 1974: Nomenclature of Corrinoids (IUPAC-IUB Commission on Biochemical Nomenclature)

Technical Reports Appendices

- No. 9, August 1974: Recommended Method for Aflatoxins in Copra, Copra Meal, and Coconut (Section on Food)
 No. 10, August 1974: Development of a Method to Evaluate Sampling Plans Used to Estimate Aflatoxin Concentrations in Lots of Shelled Peanuts (Section on Food)
 No. 11, August 1974: Collaborative Study of Determination of Aflatoxin M₁ in Milk (Section on Food)
 No. 12, August 1974: Proposed Guidelines for Testing of Single Cell Protein Destined as Major Protein Source for Animal Feed (Section on Fermentation)
 No. 13, August 1974: Report on International Education of Medicinal Chemists (Section on Medicinal Chemistry)

Comptes Rendus IUPAC Conferences*

Comptes Rendus XXVII Conference (Parts A & B), Munich (FRG), August 1973

Miscellaneous

- * International Newsletter on Chemical Education, No. 1 (November 1974)
- † International Thermodynamic Tables of the Fluid State: Ethylene 1972
- † Standard Methods for Analysis of Oils, Fats, and Soaps: Third Supplement
- † Equilibrium Constants of Liquid-liquid Distribution Reactions. Introduction and Part 1: Organophosphorus Extractants
- † Equilibrium Constants of Liquid-liquid Distribution Reactions. Part 2: Alkylammonium Salt Extractants
- † Critical Evaluation of Some Equilibrium Constants Involving Organophosphorus Extractants
- † Contributions of Chemistry to Food Supplies: Invited and Selected Contributed Papers from the IUPAC-IUFoST Symposium, Hamburg (FRG), August 1973
- † XXIV International Congress of Pure and Applied Chemistry, Hamburg (FRG), September 1973: Plenary and Section Lectures from the various Sections:

- Vol. 1—High Polymers
- Vol. 2—Chemistry of Organic Natural Products
- Vol. 3—Solid-state Chemistry
- Vol. 4—Compounds of Nonmetals
- Vol. 5—Applied Electrochemistry

*Available from IUPAC Secretariat, Oxford.

†Available from Butterworth & Co. (Publishers) Ltd., Borough Green, Sevenoaks, Kent TN15 8PH, UK.

Vol. 6—Radiochemistry

Vol. 7—Symposium on Information and Communication in Chemistry

*Advances in Mass Spectrometry, Vol. 6: Proceedings of VI International Mass Spectrometry Conference, Edinburgh (UK), September 1973

†Crystal Growth 1974: Proceedings of IV International Conference on Crystal Growth, Tokyo (Japan), March 1974

‡Proceedings of International Symposium on Macromolecules, Rio de Janeiro (Brazil), July 1974

‡Medicinal Chemistry IV: Proceedings of IV International Symposium on Medicinal Chemistry, Noordwijkerhout (Netherlands), September 1974

§Chemistry, Physical Chemistry and Applications of Surface Active Substances: Proceedings (3 Volumes) of VI International Congress on Surface Active Substances, Zürich (Switzerland), September 1972

**Nomenklatura Organické Chemie. Oddíl A, B a C—Czechoslovak version of Nomenclature of Organic Chemistry: Sections A, B, and C (3rd Edition, 1971)

††Compléments à l'Édition Française des Règles de Nomenclature pour la Chimie Organique (Sections A, B, et C)—Updating (1974) of French edition of Nomenclature of Organic Chemistry (1965)

‡‡Nomenclatura di Chimica Inorganica: Regole Definitive 1970—Italian version of Nomenclature of Inorganic Chemistry (2nd Edition, 1971)

§§Bibliography on High Temperature Chemistry and Physics of Materials:

Vol. 18, No. 1: January-March 1974

Vol. 18, No. 2: April-June 1974

Vol. 18, No. 3: July-August 1974

Vol. 18, No. 4: October-December 1974

***Bulletin of Thermodynamics and Thermochemistry—No. 17, May 1974

*Available from Applied Science Publishers Ltd., Ripple Road, Barking, Essex, UK.

†Available from North-Holland Publishing Co., Amsterdam.

‡Available from Elsevier Scientific Publishing Co., Amsterdam.

§Available from Carl Hanser Verlag, Munich.

**Available from Academia, Prague.

††Available from Société Chimique de France, 250 Rue Saint-Jacques, F-75005 Paris, France.

‡‡Available from Società Chimica Italiana, Rome.

§§Available from Dr. M. G. HOCKING, Department of Metallurgy, Imperial College of Science and Technology, South Kensington, London SW7 2BP, UK.

***Available from Publications Distribution Service, University of Michigan, 615 East University Avenue, Ann Arbor, Michigan 48106, USA.

REPORTS OF IUPAC BODIES

SECTION ON WATER QUALITY (VI.6)

Brussels, 30 June 1974

Present: Dr. S. FREYSCHUSS (Chairman), Mr. B. GÖRANSSON (Secretary), Dr. P. N. J. CHIPPERFIELD, Dr. P. R. L. A. DALQ*, Prof. E. A. PEARSON (Titular Members); Dr. E. VASSEUR (Associate Member).

1. The minutes of the previous meeting held at Munich on 23-25 August 1973 had been published in *Comptes Rendus XXVII Conference: Part B*, pp. 334-336.
2. The Section discussed and worked out adjustments to the programme of the forthcoming II International Congress on Industrial Waste Water and Wastes to be held in Stockholm during 4-7 February 1975. Preliminary selection of discussion papers to be presented was carried out. Chairmen for some of the sessions of the Congress were appointed.
3. It was agreed that an extra meeting of the Section should be held during the Congress in order to discuss the future programme of the Section.
4. It was agreed that the Section should make no comments on working papers from ISO/TC 147 (Water Quality) before all Members of the Section had submitted their considerations to the Secretary.
5. It was agreed that when reorganizing the Section consideration ought to be taken to widen the competence of the Section, especially on the analytical side.

B. GÖRANSSON

SUB-COMMISSION ON PLASMA CHEMISTRY (I.2.1)

Teddington, 5-6 September 1974

Present: Dr. D. E. JENSEN (Chairman), Dr. K. C. LAPWORTH (Secretary), Prof. P. FAUCHAIS.

The meeting was restricted to the Subcommittee formed to consider standards of measurements for plasma chemistry [see *Inf. Bull.* No. 49 (March 1975), p. 21].

It was decided that the work of the Subcommittee in the immediate future should be restricted to electrically generated plasmas at high pressures (*i.e.* *ca.* 1 atmosphere). The highest temperatures to be considered would be about 15,000 Kelvin and only 'pure' plasmas (*i.e.* single specie plasmas with no added reactants) would be considered. A report on standards of measurement for such plasmas would be prepared jointly by Prof. FAUCHAIS and Dr. LAPWORTH and would treat three topics in some detail. The first would be concerned with derivation of the volume emission coefficient throughout a plasma from sideon intensity measurements. This topic would be divided into a theoretical and an experimental part. Cylindrical and the more realistic quasi-cylindrical shaped plasmas would be considered. Various methods of solving the Abel-type integral equation would be treated. The second topic concerned the relationship between the plasma temperature and the volume

*Deceased.

emission coefficient. This would include the concept of local thermal equilibrium and its range of validity, the calculation of partition functions, and the lowering of the ionization potential in plasmas. The derivation of temperature for monatomic plasmas (with special reference to argon) and for diatomic species (with special reference to nitrogen) would be considered. The third topic of plasma standards of temperature and radiation would be concerned with recent progress and development of these devices, based on wall-stabilized arcs. The report on the Subcommittee's activities was expected to be available during the Summer of 1975.

The next meeting of the Subcommittee would be held in conjunction with the IUPAC International Plasma Chemistry Symposium to be held in Rome in September 1975.

D. E. JENSEN

SECTION ON PESTICIDES (VI.5)

Bracknell, 30 September and 4 October 1974

Present: Dr. D. C. ABBOTT (Chairman), Dr. P. SLADE (Secretary), Dr. H. FREHSE, Dr. K. R. HILL, Dr. P. C. KEARNEY, Prof. P. E. KOIVISTOINEN, Dr. J. MIYAMOTO, Dr. G. WIDMARK (Titular Members); Dr. V. BÁTORA, Dr. CH. RESNICK (Associate Members).

1. Minutes of Previous Meeting

The minutes of the meeting held in Munich during 22, 23 and 27 August 1973 (see *Comptes Rendus XXVII Conference: Part B*, pp. 250-252) were adopted with one minor amendment.

2. Matters Arising from Minutes

- (i) It had been mentioned at the last meeting that IUPAC had 'Official Consultative Status' with FAO. This had been agreed in a letter of 8 January 1973 in a letter from Dr. A. H. BOERMA, Director-General of FAO. One important outcome of this status was that the two organizations had agreed to exchange publications.
- (ii) WMO and EPPO had been invited to attend meetings of the Residue Analysis and Terminal Residues Commissions of IUPAC and joint meetings of the Commissions with the Section. WMO had declined the invitation; EPPO had accepted, but the delegate had withdrawn at the last minute.
- (iii) It had been hoped to publish the minutes and appendices of meetings of the Pesticide Commissions in *Residue Reviews*. This had not so far proved to be possible. The matter would be taken up again during the next year. Dr. FREHSE had hoped to prepare a general article on the Section and its Commissions for *Residue Reviews*, but would postpone this until after any reorganization in 1975 (see Item 3).

3. Reorganization of Applied Chemistry Division

Recent correspondence from Dr. H. EGAN indicated that after the 28th IUPAC Conference (Madrid, 1975), the Applied Chemistry Division would contain Commissions only and no Sections. There was considerable discussion about the implications of such action, and it was agreed that it would be necessary for there to be good liaison between the two Pesticide Commissions

in order to ensure continuation of some of the work now carried out in the meetings of the Section. Careful consideration was given to possible future direction of the Commissions' work which might require further reorganization. Members were asked to consider this matter before the next meeting.

4. Membership

Dr. SLADE was giving up the post of Secretary; Dr. HILL was nominated in his place. Dr. ABBOTT stressed that careful consideration would have to be given to new memberships next year in view of the reorganization of the Division. It was hoped that persons whose terms as Titular Members would be completed in 1975 would be eligible for election to the new Commissions.

5. Representation of Section at Meetings of Other Organizations

This was normally achieved by sending an appropriate IUPAC member (who would often be attending the meeting in any case). Because it was necessary to minimize the costs of such activity, on occasion a close associate of a IUPAC member, rather than a member, might have to attend, but this should happen as infrequently as possible.

6. AOAC

At the XXVII Conference (Munich, 1973) IUPAC had granted Associated Organization status to AOAC. Dr. HILL was attending the present meetings partly as an observer for AOAC as well as in his normal IUPAC role.

7. International Congresses of Pesticide Chemistry

(i) *Helsinki Congress* (July 1974). This was agreed to have been a very successful meeting and the Section thanked Prof. KOIVISTOINEN for his role in ensuring that success.

(ii) *1978 Congress*. After the last meeting of the Section, it was agreed that Switzerland would be the first choice venue for the 1978 Congress. The invitation to Switzerland had been officially accepted, and the Congress would be held in Basle in mid-July 1978.

(iii) *1982 Congress*. Dr. MIYAMOTO proposed that Japan should be the location for the 1982 Congress. This was supported, and Dr. MIYAMOTO agreed to discuss the matter further in Japan.

8. Encouraging Research in Pesticide Chemistry

Dr. RESNICK introduced an item in which discussion took place of the possibility of sponsoring an award for excellence in pesticide chemistry research or encouraging outside workers to carry out some of the research which the Commissions considered to be necessary. This would be considered further by Members during the year and discussed again at the next meeting.

9. Date and Place of Next Meeting

This would be in Madrid during 3-7 September 1975 at the 28th IUPAC Conference. The schedule adopted for the present meetings would be followed again: viz. 1 day for technical discussions by each of the Pesticide Commissions, with 1 day for a Section Meeting and 1-1.5 days for a joint meeting of the Section and its Commissions.

Dr. FREHSE said that Bayer AG (Leverkusen, Federal Republic of Germany) would be happy to act as host for the 1976 meeting.

P. SLADE

**Joint Meeting of Section on Pesticides (VI.5) with
Commissions on Terminal Pesticide Residues (VI.5.1)
and Pesticide Residue Analysis (VI.5.2)**

Bracknell, 1 and 4 October 1974

Present: Dr. D. C. ABBOTT, Dr. P. SLADE, Dr. H. FREHSE, Dr. K. R. HILL, Dr. P. C. KEARNEY, Prof. P. E. KOIVISTOINEN, Dr. J. MIYAMOTO, Prof. G. WIDMARK, Dr. V. BÁTORA, Dr. CH. RESNICK (VI.5); Prof. D. G. CROSBY, Dr. H. GEISSBÜHLER, Prof. F. KORTE, Dr. H. M. DEKHUIJZEN, Dr. N. DRESCHER, Prof. R. ENGST, Dr. R. GREENHALGH, Dr. P. E. PORTER (VI.5.1); Dr. P. B. POLEN, Mr. K. E. ELGAR, Dr. S. GORBACH (VI.5.2); Dr. S. DORMAL VAN DEN BRUEL (CEE), Dr. P. A. GREVE and Mr. A. J. PIETERS (CCPR), Dr. E. E. TURTLE (FAO).

Members stood in a silent tribute to the memory of Dr. H. HURTIG, a former Chairman of the Pesticides Section, who died at the end of 1973.

I. Nomenclature

Dr. FREHSE drew attention to the fact that Members of IUPAC bodies were sometimes expected to give advice on pesticide nomenclature in view of IUPAC activity in the nomenclature field. It was agreed that the Section and its Commissions had not the expertise to include nomenclature in their discussions.

Dr. ABBOTT said that the UK Laboratory of the Government Chemist could give advice on nomenclature and Dr. GREENHALGH indicated that Chemical Abstracts Service also gave advice on the subject. It was agreed that a multiplicity of names for compounds led to confusion, and a plea was made to minimize this: Dr. KEARNEY noted that Chemical Abstracts Service was preparing new names to aid in computerized retrieval of information. Dr. ABBOTT drew attention to a new WHO booklet on pesticides nomenclature [D. ARMSTRONG LOWE and A. R. STILES, *Bull. World Health Org.* **49**, 169 (1973)].

2. International Congresses of Pesticide Chemistry

(i) *Helsinki Congress* (July 1974). Prof. KOIVISTOINEN summarized the activities of the Congress. Some 450 papers were read (out of 539 registered) in 54 half-day sessions. He was congratulated for the efficient way in which the workload had been carried and for the overall success of the Congress. There was some discussion of what lessons needed to be learned from the Helsinki Congress which could be applied to future Congresses. Some of the points which emerged from this were:

(a) It led to considerable organizational problems when delegates registered to present papers but failed to appear at the actual Congress.

(b) In future it seemed unnecessary for every paper submitted to be read; some could be summarized into a review paper, others might be published in the proceedings of the Congress, but not presented.

(ii) *1978 Congress*. Dr. GEISSBÜHLER presented a summary of the likely topics to be included in the 1978 Congress in Basle:

- Synthesis of Pesticides (with emphasis on new synthetic methods)
- Relationship between chemical structure and biological (including toxicological) activity
- Natural products with pesticidal activity
- Degradation
- Biochemistry of pests and mode of action of pesticides (including resistance mechanisms)
- Pesticide residues (including methodology)
- Formulation chemistry (with special reference to biological effects)

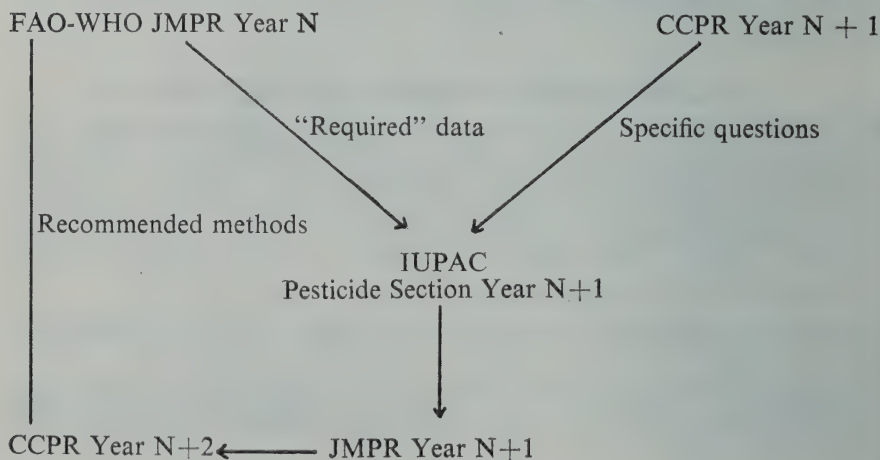
These topics were discussed and agreed to be suitable. An additional topic on Education in Pesticide Chemistry might be included.

Following a discussion of the extent to which biological matters (including toxicological ones) should be discussed at the Congress, it was agreed that to a limited extent this was desirable. The impact of pesticide chemistry on toxicology and legislation could be very important. In this connexion it was agreed that it was desirable for the Section to be represented on the Permanent Committee of the International Plant Protection Congresses.

3. Liaison with International Organizations

(i) *FAO-WHO and Codex Committee on Pesticide Residues*. The communications between these organizations and IUPAC Pesticides Section and its Commissions were discussed, with special reference to the way in which the Pesticides Section could answer questions and problems raised by the other organizations. The Minutes of the Commissions' Meetings and the relevant Appendices were sent to the organizations, but it might not always be sufficiently clear as to how the Commissions' recommendations were reached. It was also agreed that there might be an improvement in publicizing requests for work needed by the two organizations to alert universities and research institutes of possible research topics: the Pesticides Section provided a useful link in this process.

The general routes of intercommunication between the organizations was agreed to be:—



After the discussion Mr. PIETERS noted his gratitude at having had the opportunity to attend the Commissions' Meetings. He felt sure that the IUPAC recommendations were useful to the FAO-WHO Joint Meetings on Pesticide Residues (JMPR) and to the Codex Committee on Pesticide Residues (CCPR). He emphasized the dependence of legislators on scientists (in this case on residue analysts), which gave the latter the responsibility of explaining and interpreting their results. This included drawing attention to the variability of analytical figures, problems of sampling, and of the analytical procedures themselves, as outlined, for example, in Dr. FREHSE's plenary lecture presented at the Pesticide Congress in Helsinki in July 1974. All these things were related to the difficulty of setting tolerances. Mr. PIETERS hoped that the Commissions would continue to provide this type of information, and he would do all he could to promote an awareness within Codex of the IUPAC work on pesticides. He stressed the need to look ahead to attempt to forecast new developments in the field of residues. He thought that in future greater emphasis would be placed on terminal residues by JMPR and Codex.

(ii) *CEE*. Dr. DORMAL VAN DEN BRUEL also considered that the methods by which the recommendations were produced by the Commissions should be explained more fully. In a discussion on the use of 'recommended' methods for analysis, it was again stressed that the analytical expertise in any laboratory was all important, and when samples were analysed by specified methods, more variability occurred than when methods familiar in the particular laboratory were used. Dr. DORMAL said that CEE was ready to consider advice from the Pesticides Section insofar as this was appropriate for the purposes of CEE directives.

(iii) *COMECON*. It was hoped that COMECON would strengthen its links with the Pesticides Commissions. Dr. BATORA explained that COMECON had recommended analytical methods. Residue tolerances were being evolved in COMECON countries; JMPR and Codex had an important influence on this process.

(iv) *AOAC*. Dr. HILL said that AOAC would only endorse and recommend analytical methods which were supported by interlaboratory studies. Dr. W. HORWITZ of AOAC had invited a report of the present IUPAC meetings to be given at the Association's next meeting. Dr. HILL would prepare that report.

(v) *IAEA*. Although Dr. F. P. W. WINTERINGHAM had been unable to attend the meeting, the Agency still wished to keep in touch with the Commissions' work.

4. Future Changes in Organization

These had been outlined at the Pesticides Section meeting (see pp. 15-17). During the coming year, Members should give careful thought to the future structure of the Commissions and to the projects to be undertaken.

P. SLADE

COMMISSION ON TERMINAL PESTICIDE RESIDUES (VI.5.1)

Bracknell, 2 October 1974

Present: Dr. K. R. HILL (Chairman), Dr. P. C. KEARNEY (Secretary), Prof. D. G. CROSBY, Dr. H. GEISSBÜHLER, Prof. F. KORTE, Dr. J. MIYAMOTO, Dr. P.

SLADE (Titular Members); Dr. H. M. DEKHUIJZEN, Dr. N. DRESCHER, Prof. R. ENGST, Dr. R. GREENHALGH, Dr. G. E. MAYR, Dr. P. E. PORTER (Associate Members); Dr. D. C. ABBOTT, Dr. V. BÁTORA, Dr. S. DORMAL VAN DEN BRUEL, Mr. K. E. ELGAR, Dr. H. FREHSE, Dr. S. GORBACH, Dr. P. A. GREVE, Mr. A. J. PIETERS, Dr. P. B. POLEN, Dr. E. E. TURTLE, Prof. G. WIDMARK (Observers).

1. Minutes of Previous Meeting

The minutes of the Seventh Meeting of the Commission, held in Munich on 23-24 August 1973, had been published, together with Appendices, in *Comptes Rendus XXVII Conference: Part B* (see pp. 253-302). Several nomenclature corrections were noted. Dr. RESNICK reported that information on methidathion was being summarized from South African and Israeli studies and would be distributed at the next meeting. Dr. HILL was having difficulty obtaining a copy of the article by WINTERLIN and MOURES in *Pest. Monitor. J.* on azinophos-methyl, ethion, phosalone, and naled.

The Chairman would continue to publish a short report of the Commission meetings in *J. Assoc. Offic. Anal. Chem.* and he would approach Dr. F. GUNTHER about publishing the Appendices in *Residue Reviews*.

2. Organochlorine Insecticides

Dr. PORTER presented a report to the Commission on the terminal residues of cyclodiene insecticides by Prof. KORTE and himself (Appendix I). The report covered metabolic pathways, metabolites, and photoproducts of chlordane, aldrin, dieldrin, and heptachlor.

Dr. POLEN recommended that the occurrence and true significance of these products should be assessed at next year's meeting. Dr. HILL also requested an evaluation of these products in the environment to determine their toxicology. Dr. ABBOTT recommended that an authoritative article should be published on the latest advances in cyclodiene chemistry. Prof. KORTE pointed out that different results were obtained with photodecomposition on leaf surfaces and silica gel. He also pointed out that there was a need for strictly comparable metabolic studies to discover the real significance of metabolites.

Dr. HILL presented a report on terminal residues of toxaphene (Appendix II). The report covered a half-day symposium on toxaphene on 10 September 1974 at the 168th American Chemical Society Meeting in Atlantic City, New Jersey. Dr. RESNICK and Prof. KORTE requested a summary of the symposium. The symposium was organized by Dr. C. L. DUNN (Research Center, Hercules Inc., Wilmington, Delaware). Papers presented by G. A. BUNTEN (Hercules) on preparation and properties of toxaphene, and D. K. BLACK (Hercules) on composition of toxaphene were discussed by several Commission Members.

3. Organophosphorus Insecticides

Three reports on terminal residues of diazinon, Surecide, and leptophos (Appendix III) were presented by Dr. MIYAMOTO and an overview on organophosphorus insecticides by Dr. GREENHALGH (Appendix IV). Highlights of the discussion were that leptophos was fairly stable in the environment, but rapidly eliminated and metabolized in animals. Dr. GEISSBÜHLER suggested that the metabolic pathway for diazinon might have to be redrawn to include additional information. Dr. POLEN pointed out that des-bromoleptophos was an important metabolite. Dr. TURTLE again emphasized there was no signi-

ficance assigned to any of the metabolites mentioned and that no further work on diazinon was required of the Commission, because it had been reviewed and an ADI established.

4. Carbamate Insecticides

Dr. KEARNEY read salient points from a report prepared by Dr. R. L. BARON (Appendix IV). The report covered carbaryl, carbofuran, methomyl, aminocarb, mexacarb, and meobal. There followed a considerable discussion on the significance of nitrosocarbaryl and whether further study was necessary on this compound. A copy of an article entitled 'Nitrosocarbaryl as a Potent Mutagen of Environmental Significance' [*Nature* **247**, 386 (1974)] was obtained and reviewed by the group, which expressed an opinion that comments relating to the environmental significance of nitrosocarbaryl should be viewed with caution.

5. Fumigants

Dr. MAYR discussed three reports covering methyl bromide, ethylene oxide, and phosphine (Appendix VI). He drew attention to a previous report suggesting that residues from ^{32}P -phosphine in several foodstuffs were persistent and that 25% of the parent material was recovered in residue analysis. Dr. MAYR had found that impurities in the labelled materials used to prepare ^{32}P -phosphine were responsible for the reported residues in foodstuffs. Dr. HILL recommended the Pesticide Residue Analysis Commission should review and consider the second paragraph in the phosphine report.

6. Fungicides

Dr. DRESCHER reviewed a report on terminal residues of dithiocarbamates prepared by Prof. ENGST and himself (Appendix VII). The report dealt primarily with ethylene bisdithiocarbamate fungicides and the decomposition product ethylene thiourea (ETU). Prof. ENGST pointed out there were analytical problems with ETU still unresolved. He further emphasized that ETU was a product in many commonly used fungicides and its toxicology should be called to the attention of the Joint Meeting of FAO-WHO. Prof. CROSBY reported that ETU was rapidly photodecomposed and could not be detected in tomato fields in California. Also, he had found that ETU photodecomposition was accelerated in ditch water by natural sensitizers. Dr. TURTLE pointed out that a method was needed for residues in poultry and eggs. Dr. RESNICK recommended that a group be established to consider the imidazoles, and that his group was working on thiabendazole which would be reported at the next meeting. Dr. TURTLE enquired whether this new work raised any further problems. Dr. RESNICK stated that there would not be any new problems at this time.

7. Herbicides

Dr. GEISSBÜHLER presented a report on terminal residues of aniline-type herbicides and the formation of condensation products in soil (Appendix VIII). The major concern here had been the formation of azobenzenes and related condensation products when high concentrations of these aniline herbicides were applied to soils. From present evidence it was concluded that the condensation products discussed did not represent significant terminal residues of anilides, phenylcarbamates, phenylureas, and formamidines in agricultural soils.

Dr. DEKHUIJZEN reported on the uptake and metabolism of chlormequat in wheat plants (Appendix IX). Chlormequat was rapidly taken up in the wheat plant and converted to choline. The choline was further metabolized to betaine, then to glycine, serine, and carbon dioxide. Chloromequat breakdown was slow in potato and poinsettia plants. The group's attention was drawn to a publication by C. INTRIERI and K. RYSEGO entitled 'Uptake, Transport, and Metabolism of (2-Chloroethyl)trimethylammonium Chloride in Seedling of Almond' [*J. Amer. Soc. Hort. Sci.* **99**, 349 (1974)], suggesting that the compound might be an alkylating agent and consequently of some public health concern. A review of the article suggested, however, that this conclusion could not be drawn from the data presented.

8. Photodecomposition

Dr. CROSBY reviewed the photodecomposition of chlorinated pesticides, with special attention to the chlorinated aliphatic hydrocarbons, chlorinated arylalkyl compounds, chlorinated aromatic hydrocarbons, and other chlorinated pesticides (Appendix X). It was pointed out that photoreduction was important in some pesticides, *i.e.*, the replacement of Cl by H and of NO₂ by H. He pointed out that it was difficult to relate laboratory work to actual field conditions. For example, silica gel surfaces were not similar to soil surfaces. Dr. CROSBY reported that tetrachlorodioxin was stable to sunlight on soil or leaf surfaces, but in the formulated mixture some decomposition was occurring. He pointed out that the next few years would afford an opportunity for examining photodecomposition under actual field conditions.

9. Membership

Drs. HILL and ABBOTT recommended that new membership be considered at the Section meeting at Bracknell. Drs. HILL and SLADE would leave the Commission next year and, therefore, two vacancies would occur.

10. New Business

Compounds for working assignments were considered for 1975. A review of Appendix 2 of the Report of the 1973 Joint FAO-WHO Meeting (pp. 34-42) identified several compounds that required further consideration by the Commission. These included the following, with suggested reviewers:

Azinphos-ethyl—MIYAMOTO and GREENHALGH

Benomyl—GORBACH

Campechlor—HILL

Carbendazin—DRESCHER

Formothion—GREENHALGH

Hexachlorobenzene—KORTE and PORTER

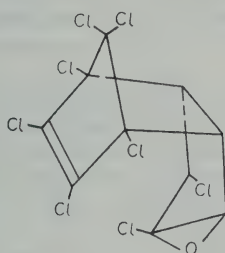
Thiophanate-methyl—MIYAMOTO

It was also recommended that the same assignments be continued for next year for those Members not covering specific subjects.

P. C. KEARNEY

Appendix I: Terminal Residues of Cyclodiene Insecticides

Interest in the terminal residues of the *cis*- and *trans*-isomers of chlordane had been stimulated by the recent development of a high purity chlordane by Velsicol Chemical Corp. This product, which had been designated HCS-3260, contained approximately 98% of a 3:1 mixture of the *cis*- and *trans*-chlordanes. Residues of the chlordane isomers themselves had been thoroughly discussed in the past, and did not appear to present problems in relation to proposed uses of chlordane. Concern had arisen, however, about the important metabolite which was commonly called oxychlordane. This metabolite seemed to have been first encountered as a contaminant in milk products from cows consuming hay containing chlordane residues [LAWRENCE *et al.* (1970); BOYD *et al.* (1971)]. Subsequently, it was found to be an animal metabolite of *cis*- and *trans*-chlordane [POLEN *et al.* (1971); STREET *et al.* (1972); DOROUGH *et al.* (1973); BARNETT *et al.* (1974)], and was identified [LAWRENCE *et al.* (1970); SCHWEMMER *et al.* (1970)] as structure I:



I. Oxychlordane

Mammalian metabolism studies with chlordane had demonstrated that both *cis*- and *trans*-isomers were rapidly converted to hydrophilic metabolites which had been characterized as mono-, di-, and tri-hydroxylated derivatives and their conjugates [POLEN *et al.* (1971); STREET *et al.* (1972); DOROUGH *et al.* (1973); BARNETT *et al.* (1974); POONAWALLA *et al.* (1964, 1971)]. These metabolites were quickly eliminated. A minor part of the chlordane isomers was converted to oxychlordane; however, the slow elimination of this metabolite gave rise to measurable tissue residues. When animals were fed *cis*- or *trans*-chlordane over long periods of time, the principal residue in tissues was oxychlordane which was stored particularly in fat. In general, the *trans*-isomer gave more storage of oxychlordane than the *cis*-isomer. Male rats stored less than female rats. When feed free from chlordane was given to rats whose adipose tissue contained oxychlordane and chlordane isomers, the compounds appeared to be completely eliminated in the form of hydrophilic metabolites. In rats, the oxychlordane elimination was similar to that of dieldrin. The rate of elimination in females was slower than in males, and in both the rates appeared somewhat faster than for dieldrin.

The animal feeding data suggested that conversion rates of chlordane to hydrophilic metabolites were proportionally greater at higher feeding levels

than at low. This was particularly evident in the results reported by DOROUGH *et al.* (1973) for cows fed HCS-3260. At average feeding levels for 30 days of 0.06-0.1 ppm, the fat storage ratio (oxychlordane in fat: chlordane fed) was about 0.25; at 1-ppm feeding the ratio was 0.16; at 10-ppm feeding the ratio was 0.10; and at 100-ppm feeding the ratio dropped to 0.0196. Similarly, milk fat after 60 days of feeding had a storage ratio (oxychlordane in milk fat: chlordane fed) of 0.34 at 1-ppm feeding, 0.21 at 10-ppm feeding, and 0.038 at 100-ppm feeding. In all cases, proportionally less chlordane was stored as the feeding level increased.

The importance of oxychlordane as a metabolite of chlordane was further increased by the confirmation and consistent finding of this compound in general population adipose tissue samples obtained through the US National Human Monitoring Programme. BIROS and ENOS (1973) examined 27 specimens and found oxychlordane contents ranging from nil to 0.40 ppm with a mean of 0.14 ppm. Twenty-one of 27 samples contained 0.03 ppm or more. Computer printouts from the EPA monitoring studies which were made available to Shell Chemical Corp., showed that in 1970 the mean oxychlordane content of human adipose tissues was 0.08 ppm with 97% of 132 samples positive (0.01 or more); in 1971 the average was 0.10 ppm with 97% of 3328 samples positive; and in 1972 the average was 0.11 ppm with 97% of 2707 samples positive.

Experiments on the fate of ^{14}C -aldrin used in the soil under simulated normal agricultural conditions, which had been in progress at the Institut für Ökologische Chemie in Federal Republic of Germany, were nearing completion. Results had been reported in past summaries and were summarized in four papers [KLEIN *et al.* (1973); KOHLI *et al.* (1973, 1974); WEISGERBER *et al.* (1974)]. A brief review followed.

In 1969, an open air experiment was started with ^{14}C -aldrin soil application (2.9 kg/ha) in several culture boxes; in 1970, one box was retreated with ^{14}C -aldrin. No further retreatment was performed since that time. Several crops had been grown each year from 1969 to 1972. The results from the years 1969 to 1970, pertaining to crop analyses and to analyses of different soil samples, had been reported last year. These studies had shown that aldrin incorporated into the soil was converted to a number of metabolites. Besides dieldrin, most of the radioactivity recovered from soils and plants was due to a group of hydrophilic metabolites. One major metabolite of this group was the dihydrochlordene dicarboxylic acid. Additionally, in the treated soils, photodieldrin and photoaldrin were also detected in small amounts, and another nonpolar component X was found but not as yet identified. In the plants, photodieldrin and component X were also found in small amounts, besides dieldrin and the hydrophilic group.

The analyses of the samples from 1971 and 1972 gave the following results: the radioactivity, as compared to earlier years, decreased in all soil and crop samples, especially in the upper soil layer (0-10 cm from surface) which had been treated; in most cases, the total residues now amounted to less than 1 ppm. While, in the first year after the application, the main portion of the radioactivity was due to hydrophilic compounds in most of the samples, in 1971 and 1972 dieldrin was the major radioactive product. A few per cent of unchanged aldrin, photodieldrin, and unidentified products were present, as well as 20-40% of hydrophilic compounds, mainly dihydrochlordene dicarboxylic acid.

The leaching water draining from the experimental boxes below 60 cm of soil was collected and also analyzed. Over a period of 3 years, approximately

10% of the initially applied aldrin was found as dihydrochlordene dicarboxylic acid in this water. The radioactivity of the leaching water amounted to 0.05 ppm in 1970 and was decreasing since that time. At the end of 1972, the water contained only 0.014 ppm of radioactivity. The radioactivity of the water contained, besides the dihydrochlordene dicarboxylic acid, very small amounts (*ca.* 2%) of *trans*-dihydroxydihydroaldrin, and traces of still unknown compounds.

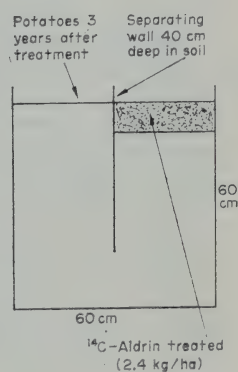
The influence of the leaching of aldrin and its metabolites on nontreated soils and crops near treated areas was investigated. ^{14}C -aldrin was applied in the open air to an area of 30×60 cm at a rate of 2.4 kg/ha and incorporated immediately to a depth of 10 cm. A nontreated area of 30×60 cm was separated from the treated area by a glass plate fixed in the soil to a depth of 40 cm. One and 3 years after application, carrots and potatoes, respectively, were planted in the untreated soil; after harvest, crop and soil samples were analyzed. The radioactivity contained the same compounds as in the other outdoor experiments described above.

Table 1 showed a survey of this experiment and its results. It showed that, after application of aldrin, aldrin and its metabolites were translocated only in very small portions to untreated soils and to crops cultivated therein.

Table 1. Lateral Movement of Aldrin

Sample	Aldrin + Dieldrin	Photo- dieldrin	Hydro- philic metabo- lites* (extracted)	Unex- tractable radio- activity	Total residue
Treated soil	0.591	0.014	0.057	0.153	0.815
Untreated soil	<0.004	<0.001	<0.001	0.004	0.008
Peeled potatoes	<0.002	<0.001	<0.001	0.001	0.001
Potato peels	<0.010	<0.005	<0.005	0.002	0.007
Potato roots	<0.186	<0.093	<0.093	0.001	0.094
Potato foliage	<0.006	<0.003	<0.003	0.011	0.014

*Principal product: Dihydrochlordene dicarboxylic acid.



The outdoor experiments of 1970 and 1971 with dieldrin were continued in 1972 with carrots as crop. The initial soil residue in 1972 was 2.628 ppm of radioactivity resulting from dieldrin treatments in 1970 and 1971. The radioactive residues in soil, carrots, and weeds consisted mostly of unchanged dieldrin, besides small amounts of photodieldrin, hydrophilic metabolites, and traces of unextractable materials. In the carrot leaves, the radioactive residues were low; the radioactive substances could not be determined separately due to the presence of high amounts of biologic coextractives.

The residues of the 1972 'dieldrin' samples are shown in Table 2.

The leaching water drained from the experimental box was collected the first year after application, and analyzed. Its radioactivity was below the detection limit (0.001 ppm). Nevertheless, it was extracted with ether after

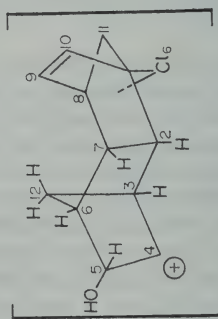
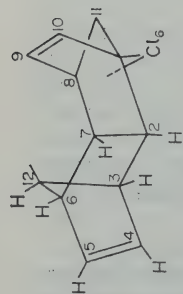
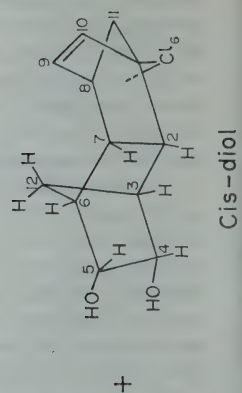
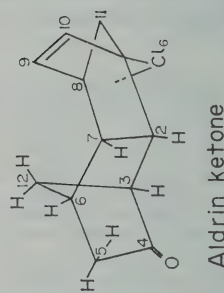
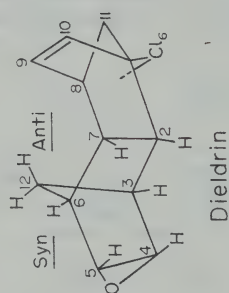
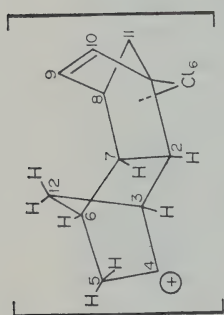
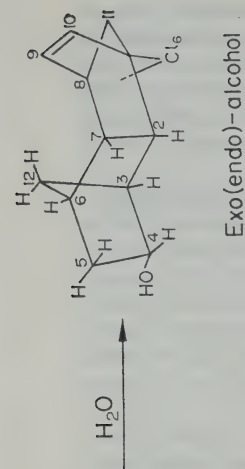


Table 2. Residues of ^{14}C -dieldrin and its conversion products in carrots and soil following soil application (expressed as equivalent ppm of dieldrin)

Sample	Dieldrin	Photo-dieldrin	Hydrophilic metabolites (extracted)	Unextractable radioactivity	Total residue
Soil, 0-10 cm depth	0.634	0.035	0.003	0.018	0.690
Carrot roots	0.125	0.005	0.002	0.003	0.134
Carrot leaves	<0.033	<0.033	<0.033	0.002	0.035
Weeds	0.343	0.045	0.006	0.007	0.401

acidification. The ether was concentrated, and its radioactivity was found to be 0.5 ppb in the water; this amount corresponded to 0.1% of the applied radioactivity. The leached metabolite was isolated; after methylation with diazomethane, it was identified by mass spectrometry, and was found to be dihydrochlordene dicarboxylic acid dimethyl ester.

Further studies in other laboratories had demonstrated the metabolism of aldrin by plants and by homogenates of plant roots. EARL and KENNEDY (1973) showed that pea plants and extracts were subject to induction of aldrin metabolizing activity. The induced enzyme system appeared to lead to production of more hydrophilic metabolites, rather than increasing the rate of epoxidation to dieldrin. MCKINNEY *et al.* (1973 a,b,c) and MEHENDALE (1973) in an important study using pea and bean root preparations demonstrated that aldrin was converted to dieldrin, *cis*-aldrin diol, *trans*-aldrin diol, the ketone isomer of dieldrin, and to the *exo*-4-hydroxy-4,5-dihydroaldrin. They found that none of the products was intermediate in the formation of the others; in particular, dieldrin was not metabolized and the *cis*-diol was not epimerized to *trans*-diol. They postulated that one enzyme was responsible for hydration of aldrin to the monohydroxy compound, and that a second enzyme produced the other four through a common intermediate as shown in Fig. 1.

MCKINNEY *et al.* (1973b) discussed the stereochemical aspects of the metabolism and toxicity of some chlorinated pesticide systems. Their experiments with mammalian tissues *in vitro* showed [MCKINNEY *et al.* (1973c)] that the *cis*-diol was a metabolite of dieldrin as well as *trans*, and suggested that the *cis* might be an intermediate in the formation of the *trans*. They demonstrated that the *cis*-diol was converted by mammalian tissue preparations to the *trans*-isomer. The epimerization was stereoselective, resulting in optical activity in the *trans*-isomer. They postulated on the basis of their evidence that the epimerization might involve the formation of α -hydroxy aldrin ketone, which was again reduced to both *cis* and *trans* diols. They observed no transformation of the *trans* diol in their system, so that the cycle of oxidations and reductions would result in conversion of the *cis*- to the *trans*-isomer but not the reverse. The possibility was not ruled out that hydroxyketone was formed directly from dieldrin by microsomal hydroxylation at one of the epoxide carbons.

An attractive scheme for metabolism of dieldrin in animals would result from hydrogen or hydride extraction, followed by introduction of hydroxyl. This proposal (by D. H. HUTSON and C. T. BEDFORD, and by MCKINNEY *et al.*) would essentially look like Fig. 2. It would account for known metabolites,

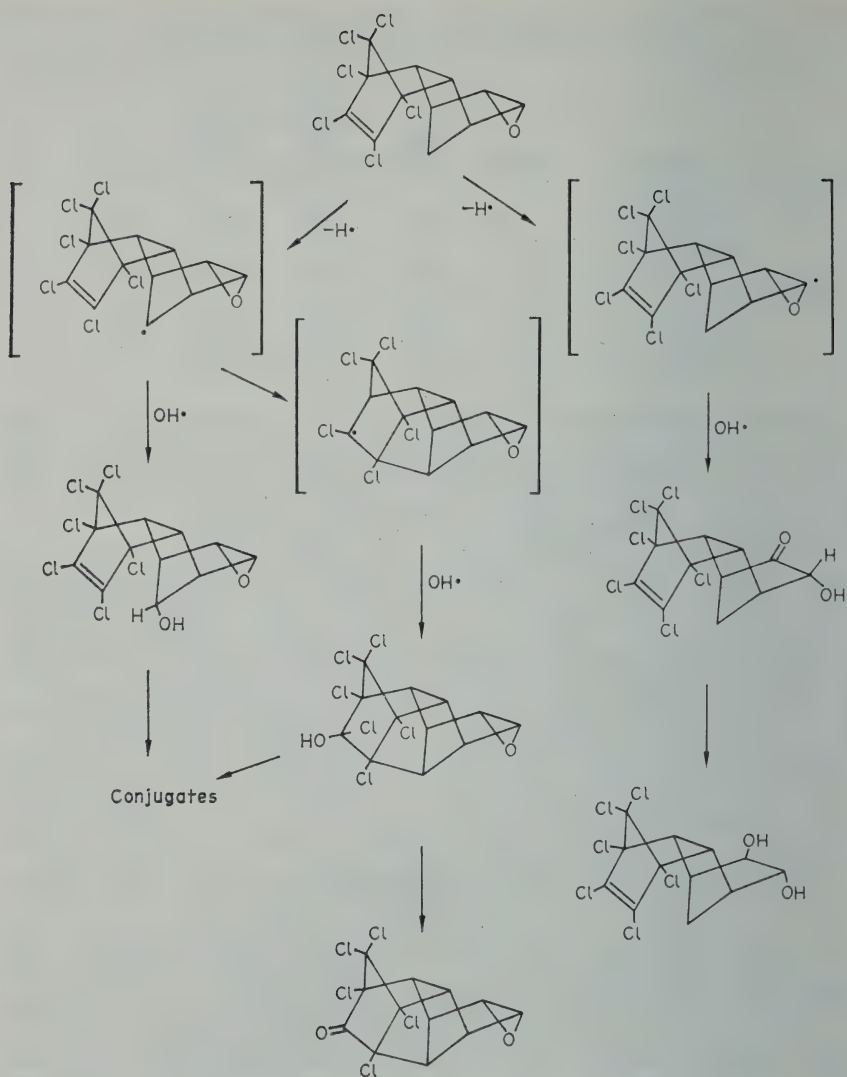


Fig. 2. Proposed scheme for mammal metabolism of dieldrin [D. H. HUTSON and C. T. BEDFORD, Tunstall Laboratory, Shell Research Ltd., MCKINNEY *et al.* (1973)]

including the glucuronide intermediate found in *in vitro* preparations by MATTHEWS and MATSUMURA (1969). This scheme was also compatible with that proposed for aldrin metabolism in plants (Fig. 1).

The Institut für Ökologische Chemie under the direction of Prof. KORTE was working on a number of aspects of cyclodiene metabolism and environmental degradation. The work on photochemical breakdown would be discussed in a later section. The following paragraphs outlined some of their recent unpublished results in other areas.

Trans-dihydroxydihydroaldrin. *Trans*-dihydroxydihydroaldrin was known to be a major metabolite of aldrin and dieldrin in mammals. Some years ago, it was shown in the Institut that it was not the end product of aldrin metabolism. After application of the radiolabelled diol to mammals, it was found to be oxidized to dihydrochlordene dicarboxylic acid; in microorganisms, too, the formation of a highly hydrophilic metabolite was observed.

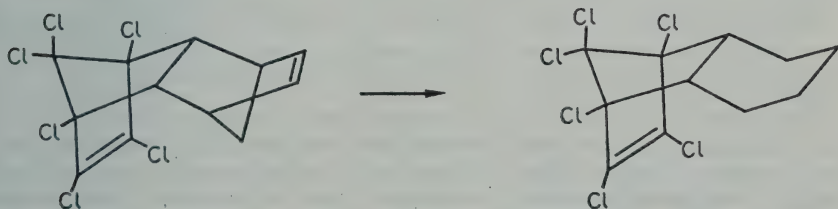
To elucidate the fate of *trans*-dihydroxydihydroaldrin in higher plants and soil, the ^{14}C -labelled compound was applied to soil and to lettuce leaves, in a plant growth chamber. In soil, more than 70% of the recovered radioactivity was due to hydrophilic compounds, mainly to dihydrochlordene dicarboxylic acid, after 7 weeks. In lettuce leaves, 4 weeks after foliar application, about 40% of the radioactivity was due to hydrophilic metabolites; the main product was again dihydrochlordene dicarboxylic acid.

Dihydrochlordene Dicarboxylic Acid. Because the metabolism experiments with aldrin and its primary metabolites resulted in dihydrochlordene dicarboxylic acid, experiments were started to find out whether this compound was indeed the final product of aldrin metabolism. The acid was synthesized ^{14}C -labelled and applied to rats, mosquito larvae, soil microorganisms, and maize. In rats, after intravenous injection, 87% of the radioactivity was excreted within 5 days. The excreted radioactivity consisted of the unchanged acid as well as of several metabolites, some of which, however, were only conjugates of the unchanged acid. The main metabolites were two isomeric dechlorination products, with dechlorination at the dichloro methylene bridge. Both isomers were also detected in *in vitro* experiments with rat-liver homogenate fractions. In smaller amounts, several breakdown products of the dihydrochlordene dicarboxylic acid with low molecular weights were detected; however, their structure could not be elucidated.

Less than 10% of the dihydrochlordene dicarboxylic acid applied to water was metabolized by mosquito larvae within 72 hours, and, also less than 10% by soil microorganisms within 3 weeks. Dihydrochlordene dicarboxylic acid was applied to the leaves of young maize plants, in a plant growth chamber, and worked up when they had developed cobs. Besides the unchanged acid, conjugates of the unchanged acid were detected, as well as conjugates of a degradation product; however, the latter substance amounted only to 2% of the total radioactivity recovered.

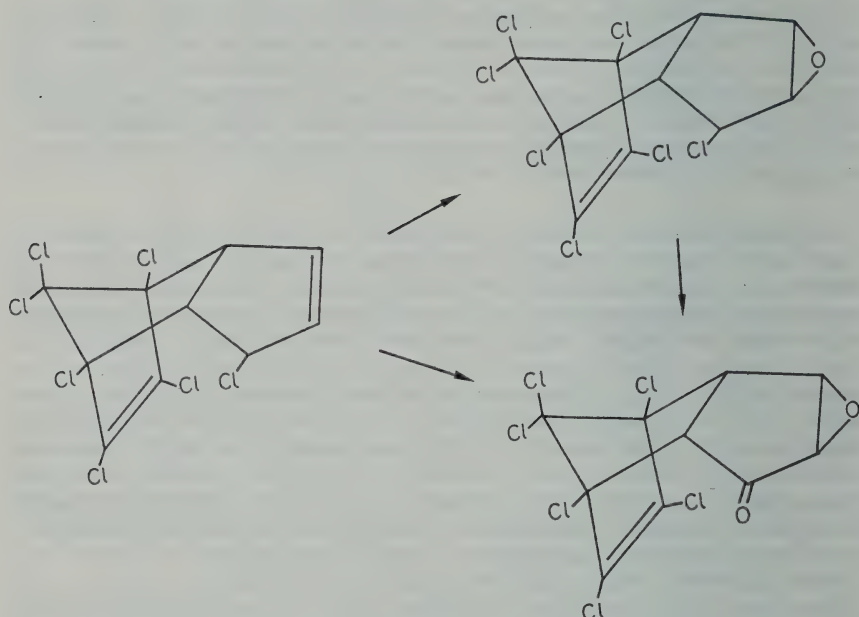
All these experiments showed that dihydrochlordene dicarboxylic acid was not the final product of aldrin metabolism, but that it was a persistent intermediate which was degraded very slowly in the environment.

Experiments with ^{14}C -Aldrin, ^{14}C -Heptachlor, and ^{14}C -Lindane in Algae



Aldrin metabolite from *Chlorella pyrenoidosa*

After application of ^{14}C -aldrin to the nutrition solution of the green alga *Chlorella pyrenoidosa* (2.5 ppm), 48% of the applied radioactivity was taken up by the algae within 14 days. About half of this radioactivity consisted of a metabolite which was identified as 1,2,3,4,9,9-hexachloro-1,4,4a,5,6,7,8,8a-octahydro-1,4-methanonaphthalene.



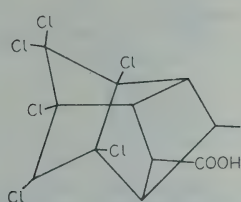
Transformation of heptachlor and heptachlor-epoxide by *Chlorella pyrenoidosa*

^{14}C -heptachlor and ^{14}C -lindane were also applied to the nutrition medium of the same green algae. With heptachlor (1-5 ppm in the medium), about 66% of the applied radioactivity was taken up by the algae within 14 days. The algae extract contained unchanged heptachlor, heptachlor epoxide, three minor hydrophilic metabolites which were not identified, and a conversion product which constituted 7% of the radioactivity detected in the algae extract. This compound was identified by mass spectrometry, and was found to be 4,5,6,7,8,8-hexachloro-2,3-epoxy-4,7-methano-3a,4,7,7a-tetrahydroindan-1-on. The same compound was detected in the algae extract after application of heptachlor ^{14}C -epoxide to the nutritive medium; thus, this compound might be formed from heptachlor via heptachlorepoide.

After application of lindane (1 ppm in the medium), a conversion product was detected in small amounts, in the medium as well as in the algae. After isolation, it was found to be 2,3,4,5,6-pentachlorocyclohex-1-ene.

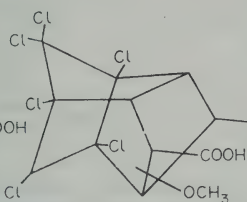
Metabolism of ^{14}C -Photodieldrin in Soil under Outdoor Conditions. ^{14}C -Photodieldrin was incorporated into the top 10 cm of soil in a tube 50 cm long and 11 cm in diameter. The tube was sunk into the soil and exposed to outdoor conditions for about 15 months. A layer of activated charcoal was placed at the bottom of the tube to prevent loss of water-soluble compounds. Overall recovery of radioactive carbon was 84.5%. In the 10-35 cm soil layers

30.2% of the radioactivity was recovered, and only 1.9% was leached to greater depth. In the 0-10 cm layer some 16.3% of the activity was in the form of metabolites and unextractables, while in the 10-35 cm layers some 25.6% was metabolites and unextractables. Three metabolites were found in the soil as shown below. The diol and the diacid were confirmed by comparison with reference standards. The third structure was proposed from mass spectra.



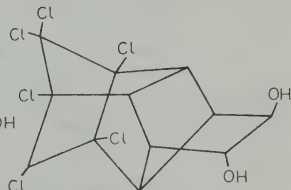
Metabolite 1—

bridged isomer of dihydro-chlordene dicarboxylic acid (MS identical to reference compound)



Metabolite 2—

bridged isomer of dihydro-chlordene dicarboxylic acid, methoxylated (structure proposal based on mass spectrum)



Metabolite 3—

bridged isomer of aldrin-*trans*-diol (MS identical to reference compound)

Results on Heptachlor. The following greenhouse experiments were carried out:

I. ¹⁴C-heptachlor was applied on the leaves of young cabbage plants (1 mg per plant, in acetone). After 4 weeks, only 7.4% of the applied radioactivity was recovered in and on the plants and 0.3% in the soil; the rest of the radioactivity probably evaporated into the atmosphere. The recovered radioactivity consisted of 7% of unchanged heptachlor, 17% of heptachlor epoxide, 6% of an unknown metabolite, and 70% of a hydrophilic group. Two components of this hydrophilic group were 1-hydroxychlordene and prillie acid.

II. Forty wheat seeds were treated individually with 11.4 µg of ¹⁴C-heptachlor in acetone and sown in a box with 21 kg of soil (intervals 5 cm, depth 2 cm). Upon harvesting (3.5 months later), 2% of the applied radioactivity was recovered in the plants and 80% in the soil. Whereas the radioactivity in the plants was too low to isolate metabolites, from the soil the following substances were isolated and identified: 18% of unchanged heptachlor, 35% of heptachlor epoxide, 12% of 1-methoxychlordene, and 35% of a hydrophilic group consisting of 1-hydroxychlordene and a monohydroxy derivative of dihydroheptachlor.

The Tunstall Laboratory of Shell Research Ltd. had recently been re-investigating the metabolism of endrin in mammals. The attached report (see p. 36) summarized its recent findings.

GRAHAM *et al.* (1973) used a potassium bromide disk technique to study the photochemical decomposition of heptachlor epoxide. They identified the structures shown in Fig. 3 as primary products in sunlight or 254 nm UV. Independently, KNOX *et al.* (1973) found these products of heptachlor epoxide. On irradiating acetone solutions of *trans*-chlordane and *trans*-nonachlor with

UV light KNOX *et al.* (1973) found new half cage isomers shown below which had different bridging than that previously observed for the *cis*-isomer.

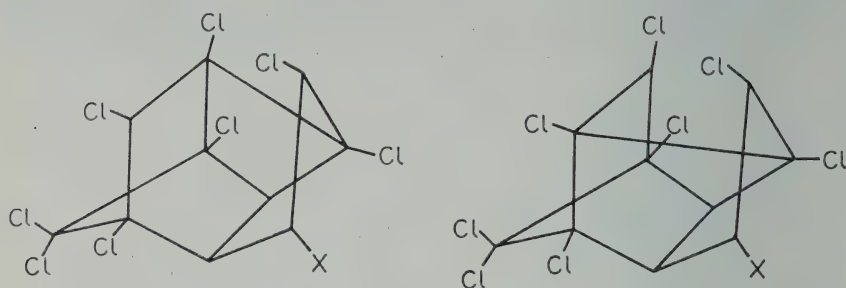


Photo-product of *trans*-chlordane (X=H) or *trans*-nonachlor (X=Cl)

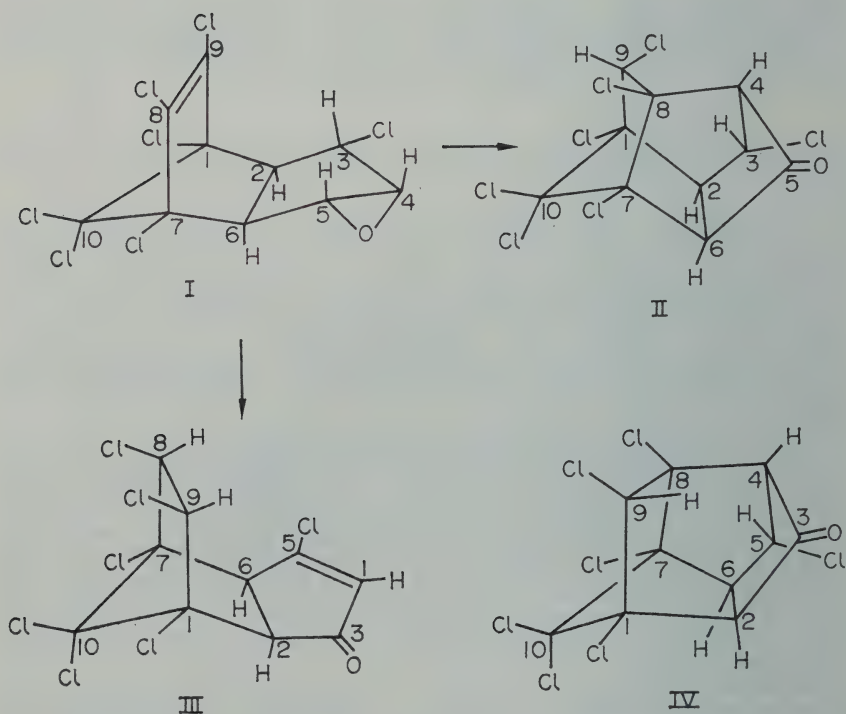
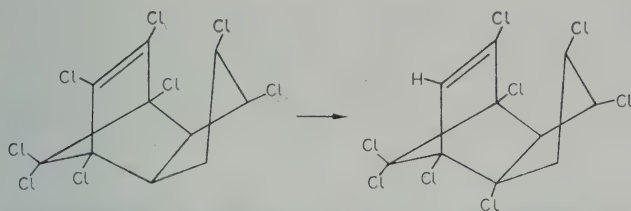
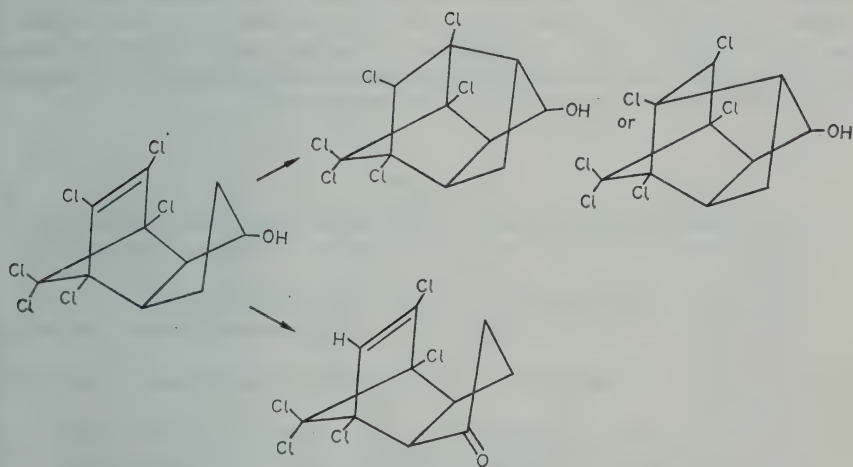


Fig. 3. Primary photoproducts from irradiation of heptachlor epoxide [from GRAHAM *et al.* (1973)]

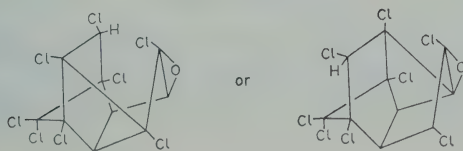
PARLAR and KORTE (1973) found that on irradiation of *cis*-chlordanes in acetone solution with light above 300 nm, the following transformation occurred in addition to the half cage structure already known:



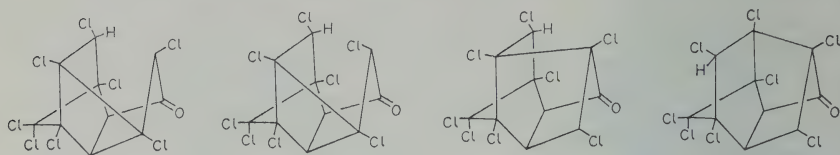
Under the same conditions 1-hydroxy-dihydrochlordene underwent the following transformations:



IVIE (1973) reported that oxychlordanes were converted into two major photoproducts when exposed to sunlight as deposits on silica gel chromatoplates. One of the products was isomeric with oxychlordanes and evidence indicated the following structure:



The other product appeared to be one or more of the following four isomers, of which the second isomer was the most likely:



The work of CROSBY and MOILANEN on vapour-phase photodecomposition of aldrin and dieldrin which was discussed in the last summary (*Comptes Rendus XXVII Conference: Part B*, page 271) had now been published [CROSBY *et al.* (1974)]. As they had pointed out, the photochemical reactions of pesticides in the vapour phase might be quite different from those occurring on surfaces or in condensed phases. It was important that both situations be studied because both conditions were represented in the environment. In this regard, KORTE and his associates had obtained evidence that aldrin, dieldrin, and photodieldrin, when adsorbed on silica gel, could be broken down completely to carbon dioxide and hydrogen chloride by light of wavelengths above 300 nm in the presence of a stream of oxygen.

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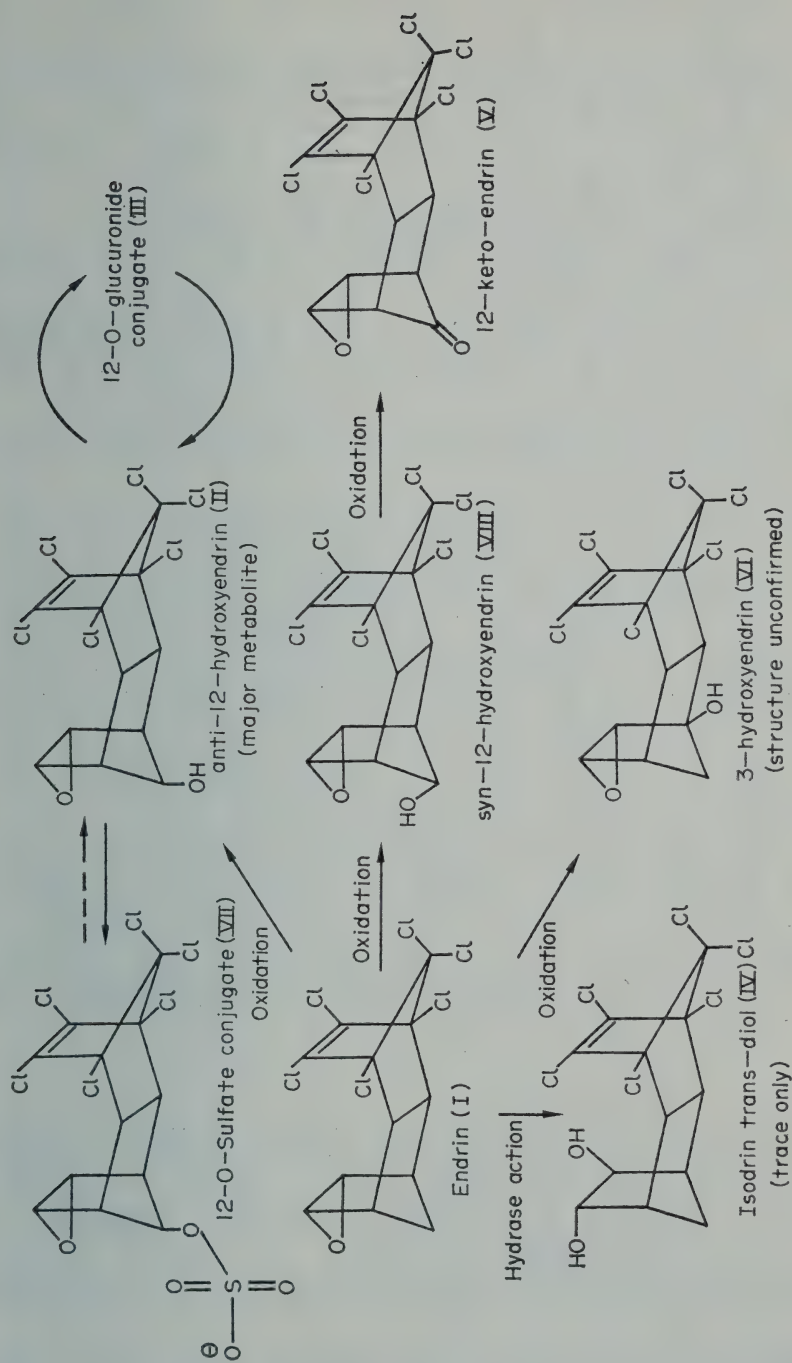


Fig. 4. Known metabolic pathways of endrin in the mammal

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*Metabolism of Endrin in Mammals in Relation to Its Acute Toxicity**

It had been known for more than a decade that endrin was readily excreted by mammals. Research by several groups in the sixties confirmed that endrin was transformed in rats and rabbits and excreted as a mixture of metabolites, but the structures of these metabolites were not elucidated. In addition, experiments in the mid-fifties indicated that the insecticide did not present a residue problem in milk when fed to cows (1). The problem was taken up in the Tunstall Laboratory in the late sixties in order to compare the metabolism of endrin with that of dieldrin, which had been under intensive study. The first information on the chemical identity of endrin metabolites in a mammal was published by Tunstall Laboratory in 1969 and 1970 (2).

Recently, there had been a reinvestigation of the metabolism of endrin in rats, rabbits, cows, and humans in relation to the industrial hygiene situation and to the consequences of an agricultural use with particular reference to metabolites rather than the parent pesticide. The studies had been aided by the recent synthesis (3) of authentic reference compounds which had not hitherto been available. Progress in the recent work on endrin metabolism was summarized below, together with findings which shed some light on the nature of the acute toxicant in endrin poisoning. Fig. 4 illustrated the structures under discussion.

Comparative Metabolism of Endrin

Rat. When endrin (I) was ingested orally by the rat (2 mg/kg), the major pathway of metabolism was hydroxylation at the 12-position to give *anti*-12-hydroxyendrin (II). This compound, probably formed in the liver, was excreted in the bile as its glucuronide conjugate (III), deconjugated by bacterial enzymes in the gastrointestinal tract, and excreted in the faeces. Endrin was also found in the faeces, together with a trace of a hydrolysis product, isodrin-*trans*-diol (IV). There was a sex difference in these processes

*Prepared by D. H. HUTSON and C. T. BEDFORD, Tunstall Laboratory, Shell Research Ltd.

in the rat. Over a 3-day period, male rats excreted 66% of an oral dose and female rats 37%. Less than 5% of the dose was excreted in the urine. This was composed of 12-ketoendrin (V), endrin (I), and 12- and 3-hydroxyendrins (II and VI), together with polar metabolites (probably the glucuronide III, the glucuronide of IV, and the sulfate VII), and traces of unknown compounds. Endrin and 12-ketoendrin were found in fat, liver, and kidney of male animals.

Rabbit. The rabbit excreted a single oral dose of endrin (2 mg/kg) in a rather different way compared to the rat. Only unchanged endrin was excreted in the faeces, mostly within 24 hours of dosing. Approximately 40% of the dose was excreted in the urine over a 13-day period. The major metabolic products in the urine were found to be *anti*-12-hydroxyendrin-*O*-sulfate (VII) and the 12-*O*-glucuronide (III). There was evidence for a small amount of *syn*-12-hydroxyendrin (VIII), both free and conjugated.

Cow. This mammal presented another excretion pattern which differed from that of the rat (though in this case the dose level used was 0.004 mg/kg/day for 21 days). About 70% of a daily dose (fed in diet) appeared in the urine and 25% in the faeces. Most of the urinary metabolite was *anti*-12-hydroxyendrin (III); traces of its isomer (VIII) and of 12-ketoendrin (V) were also found, together with some unidentified polar metabolites (*ca.* 8%) which could be the sulfate (VII). It was likely that the hydroxylated metabolites were excreted as glucuronides, which were deconjugated by bacterial β -glucuronidase in the urine. This was a feature of excretion in cows. The faecal excretion products were composed of a 1:1 mixture of endrin and 12-hydroxyendrin.

Human. *Anti*-12-hydroxyendrin (II) had been detected at low concentration in the faeces of some of a group of men working on the endrin plant at Pernis. The urine of some of these operatives contained *anti*-12-hydroxyendrin glucuronide (III). Studies had not been performed using humans under experimental conditions.

These interspecies comparisons had of necessity been made under non-identical conditions. However, in spite of differences in routes of excretion, the major metabolic step (12-hydroxylation) operated in each of the species studied. The differences that did arise were probably due to differences between the species in the biliary excretion of metabolites. There were known to be differences between rat and rabbit in the molecular weight requirements for biliary excretion of foreign compounds and, in general, lower amounts of drug and pesticide metabolite appeared in rabbit faeces. However, the extent of sulfate conjugation in the rabbit, was a unique observation.

Studies in vitro. Several of the metabolic steps discussed above were observable *in vitro* using tissue enzyme preparations. The hydroxylation of endrin could be effected by rat liver microsomes under conditions in which mono-oxygenation occurred; glucuronide synthesis had been observed using rabbit liver microsomes in the presence of *anti*-12-hydroxyendrin (II) and the glucuronic acid-donating cofactor, uridine diphosphoglucuronic acid. The hydrolysis of the glucuronide (III) had been effected by β -glucuronidase of mollusc (limpet), bovine liver, and the bacterium, *E. coli* (present in the gastrointestinal tract of rat). A particularly interesting mechanism had been elucidated for the formation of 12-ketoendrin. This metabolite was apparently *not* formed by a dehydrogenase acting on a hydroxyendrin, but via microsomal mono-oxygenation, the same process that led to the formation of *anti*-12-hydroxyendrin (II) from endrin (I). Moreover, this enzyme would convert only the *syn*-isomer (VIII) of 12-hydroxyendrin to 12-ketoendrin.

This was an interesting observation of stereochemical specificity. *In vitro* experiments had revealed a 14-fold sex difference between male and female rat liver microsomes in their ability to catalyse the reaction, the male possessing the greater activity.

Observations on the acute toxicity of endrin, *anti*-12-hydroxyendrin, *syn*-12-hydroxyendrin, and 12-ketoendrin, in male and female rats, together with analysis of certain rat tissues for these compounds suggested that:

- (a) 12-ketoendrin was probably produced *in vivo* from *syn*-12-hydroxyendrin
- (b) this reaction might account for the acute toxic effects of endrin, *i.e.* 12-ketoendrin was a toxic metabolite of endrin.

The acute toxicity to a male rat of 12-ketoendrin (1 mg/kg) and endrin (6 mg/kg) would seem to confirm the hypothesis. Thus, the same biochemical reaction which ultimately led to the detoxication of endrin (hydroxylation, which was then followed by conjugation), was also responsible for the acute toxicity of endrin to rat. The balance between the two reactions, and alterations in this balance by extraneous factors, could be critical in the onset of endrin poisoning.

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Appendix II: Terminal Residues of Toxaphene (Camphechlor)

During the past year there had been a considerable increase in research, reported or in progress, on all aspects of toxaphene chemistry. This resulted in a somewhat premature half-day Symposium on Toxaphene Composition and Environmental Fate on 10 September 1974 at the 168th ACS Meeting (Atlantic City, New Jersey). Although progress was noted, most of the work was incomplete. At this stage there was insufficient data yet to provide a complete evaluation of the mechanisms of toxaphene degradation.

Technical toxaphene had been shown to consist of at least 175 C_{10} -polychloro compounds by CASIDA *et al.* (1, 4) and KHALIFA *et al.* (2). By means of sequential liquid-liquid partition chromatography and liquid-solid adsorption chromatography, followed by preparative gas chromatography and fractional crystallization, two components of toxaphene were isolated. One component, $C_{10}H_{10}Cl_8$, comprising 6% of technical toxaphene, was 14 times more toxic to mice than toxaphene. The other component, $C_{10}H_{11}Cl_7$, 3% of technical toxaphene, was identified as 2,2,5-endo, 6-exo, 8,9,10-heptachlorobornane and was 6 times more toxic to mice than technical toxaphene.

Oral administration of ^{14}C -toxaphene and ^{36}Cl -toxaphene to rats by CASIDA *et al.* (1, 3, 4) resulted in excretion of 50-60% of the chlorine-36 in the urine and 20-30% in the faeces as chloride ion within 14 days. The tissue content of carbon-14 was very low, indicating that toxaphene components did not persist in rats.

No evidence of metabolism was detected by CARLIN *et al.* (5) when ^{36}Cl -toxaphene was applied to cotton plants maintained in a closed all-glass

system for 7 days. Residue on the plants was identified as toxaphene and the mechanism of loss was by volatilization.

Research in progress on the fate of toxaphene in soil, air, and water was reported by PLIMMER (6). Anaerobic conditions, such as in flooded soils or sediment, appeared to accelerate reductive metabolism. Otherwise, the key factors in its disappearance appeared to be photolysis and volatilization.

The following conclusions were reached at a Toxaphene Workshop (7) held in New Orleans, Louisiana, in January 1974: 'The most extensive metabolism of toxaphene seems to occur in mammalian systems where there is little apparent accumulation of toxaphene *per se*. In fish there appears to be considerable accumulation and little evidence of metabolism. Avian systems are intermediate in this respect. Our knowledge of toxaphene metabolism in mammals, birds, and fish is undoubtedly limited.'

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Appendix III: Terminal Residues of Diazinon, Surecide, and Leptophos

I. Diazinon

The mammalian metabolism of diazinon [*O,O*-diethyl *O*-(2-isopropyl-4-methyl-6-pyrimidinyl) phosphorothioate], had been studied extensively since its advent as an insecticide. In several earlier studies in the cow (1, 2) and in the goat (3), the rapid and complete elimination of the compound in urine, faeces, and milk was shown, demonstrating the urine as the main route of excretion. The fresh milk obtained from cow 0.5, 1, and 2 days after spraying with diazinon emulsion contained definite residue of diazinon with a maximum of 0.35 ppm and by 7 days the residue was the same as in milk from the control cattle (3).

The distribution and the excretion of ^{32}P -labelled diazinon was also followed in the dog (4), in the guinea pig (5), and in the rat (6). Considerable breakdown of diazinon in these species was confirmed. In the case of the guinea pig, elimination of the radioactivity ceased within 7 days, whereby more than 87% of the dose applied orally was recovered in the urine (5). In the rat (6) the biological half-life of ring- ^{14}C -labelled and ethoxy- ^{14}C -labelled diazinon was 12 and 7 hours, respectively. No cleavage of the pyrimidine ring

leading to the formation of radio active carbon dioxide occurred, whereas a small portion of ^{14}C -ethoxy (approximately 6%) was expired as carbon dioxide. The ring-radiocarbon was eliminated almost completely (95~98% of the dose) in 168 hours, with the major quantity present in the urine (80% in males and 69% in females).

Most of the urinary ^{32}P -metabolites were polar products and in the cow 50% and 45% of the urinary ^{32}P were identified as dimethylphosphorothioic acid and dimethylphosphoric acid, respectively (1). In the rat 71% of the phosphorus-32 was the phosphorothioate and 24% the phosphate (7).

The urinary and faecal radioactive metabolites of ring- ^{14}C -diazinon in the rat were resolved into four fractions by thin layer chromatography (tlc), three of which were identified by spectroscopic analysis (6). They, representing 70% of the radioactivity totally applied, were 2-isopropyl-4-methyl-6-pyrimidinol (I) and its oxidation products at the primary and tertiary carbon atom of the isopropyl sidechain (II and III). Intravenous administration of I~III revealed that II and III were derived from I, while II was excreted unchanged and III gave rise to the metabolites in fraction 4. I and III were not cholinesterase inhibitors and tenfold less toxic to rats than diazinon (6).

Several of the other ^{14}C - or ^{32}P -metabolites were separated and identified with the ester bond intact, although the quantity was presumably small in each case. The metabolites of diazinon in chloroform or acetone extract of the sheep urine were chromatographed on a silica gel column and analyzed spectroscopically in comparison with the authentic reference compounds. Thus, the structure of the three was confirmed (8, 9, 10); hydroxydiazinon or *O,O*-diethyl *O*-[2-(2'-hydroxy-2'-propyl)-4-methyl-6-pyrimidyl] phosphorothioate (IV), *O,O*-diethyl *O*-(2-isopropenyl-4-methyl-6-pyrimidinyl) phosphorothioate (V), and the 4-hydroxy analogue of diazinon (VI). Hydroxydiazinon was detected in various tissues and blood of sheep given diazinon, the amount being, however, one-tenth or less of the diazinon content. Hydroxydiazinon, V, and VI, as well as diazoxon, were demonstrated chromatographically in mice urine in *in vivo* shortly after oral administration of diazinon. The presence of the 4-formyl analogue of diazinon was presumed. V was formed also by administration of hydroxydiazinon (II). These phosphorothioate esters inhibited human plasma cholinesterase more or less similarly to diazinon and actually the oral LD_{50} of hydroxydiazinon in mice was 110 mg/kg (11), so they were likely to be toxicologically significant metabolites.

In vitro guinea pig liver slice converted diazinon to hydroxydiazinon (8). Although rat liver microsomal fractions were active in oxidatively cleaving the ester bond of diazinon, yielding dimethylphosphorothioic acid and the corresponding pyrimidinol (I) (12, 13), the similar enzyme systems oxidized diazinon to hydroxydiazinon in the presence of NADPH and oxygen (13). Also, the enzyme systems were capable of converting diazinon to diazoxon, and hydroxydiazinon to hydroxydiazoxon (VII). On the other hand, diazoxon and probably hydroxydiazoxon too, were hydrolyzed by rat liver microsomal esterase *in vitro* to yield, respectively, I and III (14). III was assumed to be derived from hydroxydiazinon also by oxidative cleavage of the ester linkage.

In the presence of reduced glutathione rat liver, the supernatant fraction transferred the pyrimidinol moiety of diazinon to glutathione to form VIII (15).

Based on these available evidences, the metabolic pathways of diazinon were as summarized in Fig. 1.

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II. Surecide

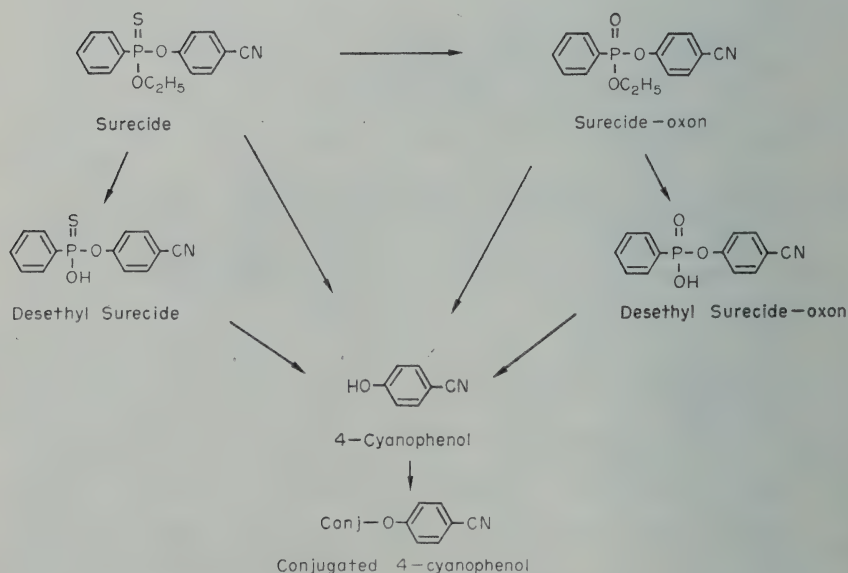


Fig. 1. Proposed metabolic pathways of Surecide (phenol moiety)

The metabolism of Surecide^{R*} (*O*-ethyl *O*-4-cyanophenyl phenylphosphonothioate) in mice (1) and in bean plants (2) was investigated with a 4-cyano-¹⁴C preparation. The proposed pathways of biodegradation were summarized in Fig. 1 and presumed to be essentially the same in both mice and bean plants.

Orally administered radiolabelled Surecide to male and female dd-strain mice was rapidly absorbed from the intestinal tract, as evidenced by the presence of radioactivity 30 minutes posttreatment in 10 major organs, fat, muscle, and blood. The tissue radioactivity was maximal 30 minutes after treatment, then decreased rapidly. In the tissues were detected such radioactive metabolites as those described below, including a trace amount of Surecide-oxon as well as unchanged Surecide.

The radiocarbons given to mice were eliminated quite rapidly, mostly within 24 hours, and during 3 days approximately 95% and 5% of the applied radioactivity were excreted, respectively, into urine and faeces. No detectable radioactive carbon dioxide was expired. The urinary radioactive metabolites of Surecide were separated and identified by silica gel tlc with authentic reference compounds. The following radioactive metabolites were presumed to be present: unchanged Surecide (5% of the urinary radiocarbons), desethyl Surecide (10%), and free 4-cyanophenol (15%). No Surecide-oxon was detected and desethyl Surecide-oxon was not confirmed positively. The polar radioactive products, amounting approximately to 70% of the urinary radioactivity, were acid-labile and by aryl-sulfatase digestion yielded mainly 4-cyanophenol.

These biodegradation patterns appeared to be essentially similar to those of the corresponding *O*, *O*-dimethyl phosphorothioate ester of 4-cyanophenol (Cyanox^{R†}) in rats (3) and Surecide was likely to be quite rapidly metabolized in mammals like another phosphonothioate insecticide leptophos (4).

The plant metabolism of radioactive Surecide was preliminarily studied in bifoliated bean plants (*Phaseolus vulgaris*, L.) under greenhouse conditions. The radioactivity was neither taken up from the root to aerial parts, nor was the radioactivity applied onto the surface of the leaf translocated to untreated parts.

Surecide seemed to be rather resistant to decomposition or volatilization under the experimental conditions. In the plant samples obtained 2 weeks after leaf application, more than two thirds of the total radioactivity and 50% of the Surecide applied initially were present. In contrast, less than 5% of the radiocarbons of Cyanox remained under similar conditions (2). The persistence of Surecide compared to Cyanox was observed in several field samples, including rice grains, vegetables, and fruits (5).

In acetonitrile extractable radioactivity 4-cyanophenol and desethyl Surecide-oxon were detected by tlc. However, neither Surecide-oxon nor desethyl Surecide had been positively confirmed.

Thus, Surecide could be regarded as a persistent, biodegradable compound and it was possibly useful as a residual insecticide without the problem of biomagnification in the food chain.

*Registered trade name by Sumitomo Chemical Co. Ltd.

†Registered trade name by Sumitomo Chemical Co. Ltd.



Fig. 1. Metabolic pathways of leptophos in mice and in cotton plants

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III. Leptophos

The metabolism of leptophos (*O*-methyl *O*-4-bromo-2,5-dichlorophenyl phenylphosphonothioate) in mice and in cotton plants was investigated with two different radiolabelled preparations (^{14}C -phenoxy and ^{14}C -phenyl) (I). The metabolic patterns were as summarized in Fig. 1 and were demonstrated to be essentially the same in both mice and in cotton plants.

Orally administered radiolabelled leptophos to female Swiss mice was rapidly degraded and eliminated. The biological half-life of ^{14}C -phenoxy was 7 hours and the elimination of radiocarbons was virtually complete 48 hours after administration. In comparison, ^{14}C -phenyl was excreted at a slower rate and the radioactivity was detected in the urine as long as 144 hours post-treatment, although the recovery of radioactivity was close to completion. The urine contained major portions of the radioactivity (90-96% of the recovered radiocarbons). In faeces there were present a small amount of intact leptophos and a trace of leptophos-oxon (less than 1% of the recovered radioactivity).

With phenoxy-labelled leptophos, more than 90% of the urinary metabolites was in the form of conjugated 4-bromo-2,5-dichlorophenol (V), although approximately 7% of the free radioactive phenol (IV) was also present. The exact nature of the conjugates was, however, not established but both enzymatic (β -glucuronidase/arylsulfatase) digestion and acid hydrolysis yielded only the phenol (IV).

The phenyl-labelled leptophos gave *O*-methyl phenyl-phosphonothioic acid (I) as the principal degradation product (*ca.* 57% of the recovered radioactivity), and as minor products *O*-methyl phenylphosphonic acid (II) and phenylphosphonic acid (III) of nearly the same amount. These metabolites were present entirely in the urine.

The unidentified product(s) was detected cochromatographing with an authentic sample of *O*-(4-bromo-2,5-dichlorophenyl) phenylphosphonothioic acid.

Thus, the metabolic pathways of leptophos in mice in Fig. 1 were similar to those proposed for other organophosphorus esters in mammals, such as bromophos (2) and ronnel (3).

The radioactive leptophos applied to the leaf surface of young cotton plants under greenhouse conditions did not penetrate into the leaf tissues, but remained on the surface and was gradually lost mainly due to volatilization. For example, 73-75% of the applied radioactivity was recovered 1 week after application compared to 11% after 9 weeks. Relatively small amounts of radioactivity were found inside the leaf as benzene or methanol extracts, or bound to the pulp.

The major radioactive compound recovered 1 week after application was unchanged leptophos (91-96%) and the amounts gradually decreased with time to approximately 29% in 9 weeks. Most of the leptophos remained on the surface, although a significant but small amount was evidently absorbed

into the leaf. Little, if any, leptophos-oxon (less than 0.1% of the applied radiocarbon) was occasionally detected at sampling periods. The alteration products such as I, II, III, and IV were demonstrated. Among the acids III was predominant with the later time. No conjugated phenol but a salt of the phenol was present. A small amount of the radioactivity from both labelled-leptophos was bound to the pulp.

Because of the stability against degradation on and in cotton plants, together with rapid metabolism in mice, leptophos could be regarded as a persistent, biodegradable organophosphorus insecticide chemical.

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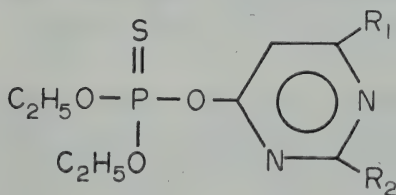
Appendix IV: Terminal Residues of Organophosphorus Insecticides

In Animals. LICHTENSTEIN *et al.* incubated ^{14}C -(2,6 ring)-parathion and paraoxon with highly purified subfractions of rat liver mitochondria and microsomes, and showed that different enzymes were responsible for degradation and detoxication. Both parathion and paraoxon were primarily degraded by the soluble enzyme fraction (105,000-500,000 g) to water-soluble metabolites together with small amounts of aminoparathion and aminoparaoxon, respectively. The microsomes showed some activity in degrading parathion. Paraoxon was degraded to 4-nitrophenol by particulate associated enzymes.

FUHREMAN *et al.* showed that ^{14}C -(ring)-parathion and paraoxon in blood were rapidly degraded by isolated perfused rat livers. Parathion degraded to give 68% of the carbon-14 as water-soluble metabolites and 2.5% converted to organic-soluble paraoxon and traces of 4-nitrophenol. Paraoxon gave 98% water-soluble products, none of which were toxic to mosquito larvae.

POTTER *et al.* administered ^{14}C -dichlorovos formulated as slow release PVC pellets to pigs, and recovered 62% of the carbon-14 as pellets in the faeces, 5.6% in the faeces, 3.6% in the urine, 14% in expired air, and 9.6% in the carcass. The dichlorovos level in the tissues ranged from 2 to 33 ppm, no demethyldichlorovos, dichloroacetaldehyde nor dichloroacetic acid were found.

JANES *et al.* dosed sheep with diazinon (1000 mg/kg) by stomach tube and characterized four metabolites found in blood, urine, and tissues. Hydroxydiazinon (I) was found in blood to the extent of 25-75% of diazinon, but less in other tissues. The amounts of metabolites II and III were small and not estimated. The compounds were distributed in tissues according to their relative polarity, diazinon and III were found in fat, and II mainly in the urine. Compound IV was only obtained by UV irradiation.



	R ₁	R ₂
I	CH ₃	C(OH)(CH ₃) ₂
II	CH ₂ OH	CH(CH ₃)
III	CH ₃	C(CH ₃)=CH ₂
IV	CH ₃	COCH ₃

In Plants. HOSOKAWA and MIYAMOTO found that ^{14}C -fenitrothion disappeared rapidly from the surface of apples, 3.95 down to 0.21 ppm in 21 days. The major degradation products on the surface were fenitrooxon, which reached a maximum of 0.017 ppm after 3 days, 4-nitrocresol, and some *S*-methyl fenitrothion. In the apple pulp, the water-soluble metabolites gradually increased with time, these including desmethyl fenitrothion and 4-nitrocresyl β -glucoside.

GREENHALGH *et al.* studied the uptake of fenitrothion by germinating pine seeds and showed that it was translocated into the embryo through the seed coat and endosperm. Metabolic products were detected in the embryo after 8 days. Desmethyl fenitrothion (25 ppm) was the main metabolic product and also postulated as a precursor for the *S*-methyl fenitrothion. Other metabolites included fenitrooxon and *S*-methyl fenitrothion present in amounts of 2.1 and 2.4 ppm, respectively, after 14 days.

CHIBA *et al.* applied topically ^{14}C -Cyanox (cyanophos) to bean leaves and found that it was translocated to all parts of the plant. Cyanophos disappeared rapidly from the leaves, 106 down to 3.5 ppm in 7 days, giving desmethyl cyanophos as the major metabolite, together with cyanophosoxon, desmethyl cyanophosoxon, and 4-cyanophenol. Stem injection of cyanophos gave the same metabolites, whilst cyanophosoxon gave only desmethyl cyanophosoxon and 4-cyanophenol.

CHIBA *et al.* also showed that ^{14}C -Suricide (cyanofenphos) was more stable than cyanophos on bean leaves, 74% remaining after 1 week and it was not translocated. Two metabolites, desethyl cyanofenphos and 4-cyanophenol were isolated, but no cyanofenphosoxon. Injection of the oxon into the stem, indicated rapid decomposition to desethyl cyanofenphosoxon and 4-cyanophenol.

LARONSON and BEN AZIZ determined the persistence of leptophos on tomatoes and grapes. Some 20% was lost in 3 weeks from tomato leaves and from 12 ppm down to 7.5 ppm in 44 days on grapes. No accumulation of the oxon analogue was found, but the phenol was present to the extent of 1-10% of that of the parent compound. There was no translocation from leaves to fruit in grapes.

Soil. SETHURATHAN examined the persistence of parathion in five acid soils and showed that rapid decomposition took place in flooded soils with a high organic content due to biological data. The rate of hydrolysis to *p*-nitrophenol was enhanced by repeated addition of parathion. A *Bacillus sp.* capable of decomposing 4-nitrophenol was isolated from parathion treated soil. SETHUNATHAN and YOSHIDA also found that the enhanced rate of parathion disappearance to give aminoparathion occurred under submerged conditions in four Phillipino soils. Soils innoculated with *Flavobacterium sp.* exhibited a high capacity for the conversion of parathion to aminoparathion.

WALKER and STOJANOVIC tested 18 soil bacteria in a mineral salt medium for their ability to utilize malathion. The *Arthrobacter* species were the most effective in degrading malathion, giving malathion half ester, malathion dicarboxylic acid, potassium dimethyl phosphorothioate, potassium dimethyl phosphorodithioate, and one unidentified metabolite. Potassium desmethyl malathion was also produced, but a nonbiological mechanism was involved.

TAKIMOTO *et al.* found that ^{14}C -(3-methyl)-fenitrothion was converted to aminofenitrothion as a result of microorganisms in four different submerged soils. Aminofenitrothion was found in 50-70% yield in 10 days. Some ^{14}C -carbon dioxide was detected from oxidation of the ring methyl group.

CHIBA *et al.* attributed the difference in the loss of radioactivity between ^{14}C -cyanophos treated soil (6% of carbon-14 remaining after 6 weeks) and ^{14}C -cyanofenphos (53% remained after 3 weeks), to differences in the volatility of the two insecticides.

Photodecomposition. OHKAWA *et al.* irradiated Sumithion (fenitrothion) with UV light in various solvents in the presence of air. The solvent determined the rate of decomposition and the products formed; the main product was carboxy fenitrothion (I) together with fenitrooxon (II), carboxy fenitrooxon (III), 3-methyl-4-nitrophenol, and 3-carboxy-4-nitrophenol. Exposure of an aqueous solution of fenitrothion (14 ppm) to sunlight gave the same products plus some *S*-methyl fenitrothion (IV). UV irradiation of fenitrothion on silica gel plates gave metabolites I, II, III, and IV, in sunlight and some 3-carboxy-4-nitrophenol was also obtained. These results corresponded closely with the effect of sunlight on ^{14}C -fenitrothion treated bean leaves, except for the absence of carboxy fenitrooxon. After 6 days, only 0.5% of the recovered radioactivity was fenitrothion.

Independently, GREENHALGH isolated 10 photodecomposition products of fenitrothion. In methanol, the main product detected by gas chromatography was carbomethoxy fenitrothion (V); in addition to the other compounds mentioned above, formyl fenitrothion (VI) and *O*,*O*-dimethyl-*O*-3-methylphenyl phosphorothioate (VII) were identified.

	Product	R ₁	R ₂	X	R ₃
I	COOH		NO ₂	S	CH ₃ O
II	CH ₃		NO ₂	O	CH ₃ O
III	COOH		NO ₂	O	CH ₃ O
IV	CH ₃		NO ₂	O	CH ₃ S
V	COOMe		NO ₂	S	CH ₃ O
VI	CHO		NO ₂	S	CH ₃ O
VII	CH ₃		—	S	CH ₃ O

JOINER and BAETCKE (1973) applied ^{14}C -parathion to cotton leaves in laboratory and field conditions. After 28 days, only 11-15% of the total ^{14}C -activity applied was recovered and found to be 58-68% unchanged parathion. Photoalteration products present included paraoxon, *S*-ethyl parathion, *S*-phenyl parathion, and 4-nitrophenol.

JOINER and BAETCKE (1974) showed that the UV irradiation of parathion (neat) for 35 days induced the formation of 15 products, 12 of which they characterized. Apart from the 4 products mentioned previously, 4-amino parathion, diethyl phenyl phosphate, *O*,*O*-diethyl-*O*-phenyl phosphorothioate, ethyl bis (4-nitrophenyl) phosphate, *O*-ethyl *O*,*O*-bis(4-nitrophenyl) phosphorothioate, diethyl phosphate, and monoethyl phosphate were identified.

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Appendix V: Terminal Residues of Carbamate Insecticides

Several reviews on carbamate metabolism had appeared recently in the literature. Two reports presented initially in 1971 at the II IUPAC International Pesticide Congress (Tel Aviv) had been published in their entirety (1, 2) and one new report on carbamate metabolism had appeared (3).

New terminal residues reported for carbaryl included a suggestion of a highly mutagenic derivative, nitrosocarbaryl, which might be formed by the interaction of nitrate and carbaryl (4, 5). It had been suggested that the compound would also be carcinogenic, based on a similarity of structure to *N*-nitrosomethylurethane. Previous studies reporting an N-O-conjugate of carbaryl appeared to have been resolved with the consideration that there was small possibility for such a reaction. The significance and actual presence of nitrosocarbamates needed to be resolved.

The metabolism of carbofuran in mugho pine, qualitatively the same as in a model ecosystem, had been reported for other organisms (6). Carbofuran was metabolized slower in the pine than in other plants and animals, and again apparently yielded 3-hydroxycarbofuran, 3-ketocarbofuran, and cleavage products. Studies designed to evaluate the interaction of carbofuran with herbicides showed that atrazine enhanced the toxicity of this carbamate to insects (7) and that its metabolism in barley was inhibited by chlorobromuron (8).

The metabolism of methomyl in rats, plants, and soil had been reported in depth (9-12). The primary metabolic pathway of methomyl followed a different pattern of metabolism from that of other oxime carbamates. No residues of the corresponding *S*-oxide or *S,S*-dioxide were observed. In plants, methomyl was converted rapidly to acetonitrile and carbon dioxide without accumulation of detectable intermediates. Reincorporation of these fragments into natural components, such as lipids and tricarboxylic acids, was demonstrated. In rats, methomyl was rapidly eliminated from the animal body in the ratio of one part of carbon dioxide to two parts of acetonitrile to one part of urinary metabolite. In soils, methomyl was hydrolyzed to the corresponding oximino compound, followed by total decomposition to carbon dioxide without formation of acetonitrile. Aldicarb, as previously reported and confirmed, followed a different pathway of metabolism and yielded a sulfoxide and sulfone prior to total degradation (12).

m-Tolyl *N*-methylcarbamate was widely used in Japan for insect control on rice. The metabolism of the compound in rats was different from most

carbamates in that there was very little hydrolysis, less than 5% of an oral dose, and that 70% of the urinary metabolites were in the free form (13, 14). The predominate metabolites in the urine were free 3-carboxyphenyl *N*-methylcarbamate and conjugated 4-hydroxy-3-methylphenyl *N*-methylcarbamate. There was almost quantitative excretion of the dose within 24 hours by male rats but only 75% by females. However, there were no differences in the nature of the metabolites in the urine of males and females.

When applied to bean leaf surfaces, there was rapid loss of the insecticide, 86% after 1 day, and little metabolism. No hydrolysis products were detected and only small amounts of carbamate-type materials. Oxidative metabolites formed by rats, houseflies, plants, and by photolytic reactions (15) were less potent anticholinesterase agents than the parent compound.

An *in vitro* artificial oxidation system was found to degrade aminocarb (Matacil) through demethylation and hydroxylation of the aromatic ring, oxidation of the methyl to the corresponding methylol, and cleavage of the carbamate to its phenol. All these reactions were similar to those previously described for the biodegradation of aminocarb and other carbamate insecticides (16, 17). Further studies on methiocarb (Mesurol) reconfirmed the metabolic pattern reported previously (oxidation, hydrolysis, *etc.*) (18).

Mexacarb (Zectran) was decomposed photolytically (296.7 nm wavelength) in solution to yield 4-dimethylamine-3,5-dimethylphenol; 4-hydroxy-2,6-dimethyl *N*-methylbenzamide; and 4-monomethylamine 3,5-xylyl methylcarbamate. This study suggested that new and previously unknown materials might occur in the environment as a result of photolytic degradation (19). In studies with meobal, the photolytic products included: 3,4-dimethylphenol; 2-hydroxy-4,5-dimethyl-*N*-methylbenzamide; and 2-hydroxy-5,6-dimethyl-*N*-methyl benzamide (20). Aminocarb was found to decompose to dimethylamino-3-methylphenol. Landrin decomposed to the trimethylphenol (21). In these studies the *in vitro* photoproduct did not correspond to photoproducts found on beans sprayed and exposed to sunlight.

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Appendix VI: Terminal Residues of Fumigants

I. Methyl Bromide

Methyl bromide had been known generally as one of the most important fumigants for many years. In the Federal Republic of Germany, about 50% of all mill fumigations were carried out with this fumigant, as were fumigations of stacked boxes and sacks and grain ships (1). BURNS BROWN had described the technique of fumigating under gas-tight sheets (2). The fumigation of flour, particularly when this was carried out repeatedly, led to complaints concerning the odour; however, because treated flour was mixed with several times its volume of untreated flour, the influence of a single fumigation was slight and never gave rise to complaints (3). It must be emphasized that methyl bromide, unlike other gases, had no narcotic effect and that there was usually a considerable difference between the dosis tolerata for plant life and the dosis letalis for pests. Absorption was slight except in substances which contained fats (4). Because the gas was highly dangerous, HUNOLD and PIETRULLA (5) had discussed methyl bromide from the point of view of work hygiene and stated the main safety precautions which had to be observed in handling the gas; also they had given methods of determining the presence of the substance in air and detecting it with a halide test lamp. The best monograph on methyl bromide was that written by THOMPSON (6), which gave details of its properties, the various applicational fields, and fumigation techniques, appropriate safety precautions, and analytical methods of determining concentrations and residues.

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II. Ethylene Oxide

Ethylene oxide was an excellent fumigant for the destruction of pests of all types—from insects through bacteria to viruses and phagocytes—in both their vegetative and permanent forms. However, because it was highly toxic for mammals and in particular humans, suitable precautions must be taken and its application should only be carried out by trained staff. One attempted to prevent the formation of explosive gas-air mixtures by adding inert gases (carbon dioxide, freons, *etc.*), but this method had proved inadequate because these mixtures could also be considered as inflammable over a wide range. Real safety was offered by the vacuum process in which the formation of explosive ethylene oxide-air mixtures was prevented from the very outset. An important feature was the high rate of penetration through all conventional packing materials so that it was possible to pack the goods bacteria-tight, to sterilize them, and subsequently to store them in a sterile condition with undamaged packaging. Being a readily reactive substance, ethylene oxide formed compounds with practically all organic substances so that undesirable reaction products could occur. Thorough chemical and physical, medical or organoleptic tests were therefore necessary (1).

In the Federal Republic of Germany, the laws which were passed concerning the use of ethylene oxide in controlling plant and animal pests also applied in connexion with its application for sterilizing purposes, an application which had been steadily increasing in significance over recent years. More modern laws of the individual Federal States were being prepared: in Bavaria they had already been in force since 1969 (2). The equipment for sterilizing with ethylene oxide was described at a symposium of the British Pharmaceutical Society (3). Numerous publications emphasized the importance of the minimum moisture content of the goods which were to be treated; sterilization would not be possible without this moisture. Equally important was 'pre-climatizing'. The moisture content of the ambient air, on the other hand, had practically no effect on the success of the treatment (1, 3, 4, 19, 20, 27, 28, 29). Among the goods sterilized were dry gelatine (5), dried egg powder (6), dried therapeutical plants and herbal preparations (7), glass, plastics, rubber, wood, cellulose, paper, linen, metal, nutrient mediums, reagents, sausage skins, meat, sausage mix (8), membrane filters, nutrient cardboard (9), and medical instruments (10). *Salmonella* and enterobacteriaceae which were found in large numbers in dried egg products, coconut scrapings (11) and bone meal (12) before fumigation, were no longer detectable thereafter. Infected shoes and stockings, and also the insoles which were practically inaccessible for fungicides, were sterilized without damaging the leather (13).

There was a particularly extensive literature concerning the cold sterilization with ethylene oxide of spices, three quarters of which were bacteriologically highly impure (14, 15). After fumigation, the residues generally disappeared after 2-3 weeks or were unimportant, because the spices were always used in great dilution (in exceptional cases, 50-100 ppm were still found). The flavouring capacity, aroma, and colour of the spices remained practically unchanged, with the exception of mustard (16, 17). In the case of black pepper, its origin (probably as a result of differing composition), grain size, and water content, and the load factor of the fumigation chamber, determined the distribution of the ethylene oxide.

The residual quantity increased parallel to grain size, as did the metabolized component; at higher water contents one found smaller residues, whilst the metabolized component changed only little. In unventilated pepper, one still

found 1,773-1,865 ppm whereof 24.6% reacted with the substances of the residue (cellulose), 11.8% with those of the water extract (sugar, proteins, amino acids), a further 2.6% with the starch, 1.3% with the dichloromethane extract, and only 0.05% with essential oils. Some 54.6-57.3% formed volatile metabolites, mainly ethylene chlorohydrin (657-761 ppm). Under practical conditions, the values were considerably lower (total quantity 866.9 ppm, reactions with 11.6%, 4.8%, 1.9%, 0.8%, and 0.4%, respectively. Some 52.6% or 456 ppm were bound adsorptively, 27.9% were volatile metabolites (ethylene chlorohydrin 302 ppm) (32). If changes in colour, pH value, *etc.*, were feared, they could be prevented by the use of ETOXIAT (a mixture of ethylene oxide and methyl formiate 1:1); the residue problem was also reduced by this method (18).

About 7 ppm of ethylene oxide were found in wheat after fumigation of a silo. Control experiments confirmed that damp wheat absorbed more ethylene oxide than dry wheat. One assumed a certain distribution of the ethylene oxide between the phases 'gas space' and the water contained in the wheat; the coefficient of distribution was determined as a special material constant of the wheat, which depended on the water content. One could then formulate a relationship which formed the basis for calculating the metabolizable or already metabolized components of the ethylene oxide in the wheat. These components depended on the water content of the grain, the distribution constants, the intensity of ventilation, the duration of ventilation, and the quantity of ethylene oxide which was employed.

The problem of residual ethylene oxide was only small from the toxicological and food law aspects, because the foreign substance disappeared through metabolism after 4-6 weeks; *e.g.*, residual analyses could no longer determine, after this time, whether a given sample had been fumigated or not. Fumigation with radioactively marked ethylene oxide and determination of the concentration through radioactivity measurements showed that there was a certain linear regression between the ash content of the flour fractions and the ethylene oxide content (bran 54 ppm; white flour 6.8 ppm; wheat germ 62 ppm; mean residue 12-15 ppm) (19-21). A comparison between the employed and recovered ethylene oxide via radioactivity measurements revealed that between 22.8% and 28.0% of the employed ethylene oxide was metabolized, thus confirming the results of earlier experiments (27.9%) (19-21). About 75% of ethylene oxide in the grain react with the water-soluble components or with the moisture content of the individual grain; approximately 28% of this reacted with water to form ethylene glycol, about 15% reacted with the water-soluble substances of albumes, about 16% reacted with the saccharides, about 12% with organic acids, and about 4% with minerals and vitamins. The majority of these reaction products were physiologically compatible. After conventional fumigation, about 11-14 ppm of the relatively toxic ethylene glycol were found; on the other hand, about 3-4 ppm of the more toxic ethylene chlorohydrin were detected. The activity of the dehydrogenase was reduced only by quintuple overdosing (30).

Also in the case of cocoa powder, the metabolism rate of ethylene oxide apparently depended on the moisture content of the foodstuff; the residual values were in reversed proportion to the water content. The water content, however, exerted no influence on the quantity of the metabolized ethylene oxide which under practical conditions was on average 11.5% of the employed quantity, but which increased with greater concentrations. From this, one could conclude that cocoa powder had an adsorption mechanism and not a distribution mechanism, as was the case for wheat. If the reaction products

were extracted, one found the toxic substances—ethylene glycol and ethylene chlorohydrin—which might have been formed, in the ether extract only, namely 9.7 ppm or less than 1.5%. In the chloroform extract one found 155 ppm, in water extract 421 ppm, and in the residue 105 ppm of metabolites. The metabolized component of the original weight of cocoa was on average 690 ppm (31).

If tobacco was fumigated with ethylene oxide to denicotinize it, an *N*-hydroethyl compound was formed (22); however, the reduction of the nicotine content was only slight (0.02-0.12%). Nicotine in the smoke, dry condensate, and benzopyrene content did not differ significantly from those of untreated samples (23). Only after treatment under extreme conditions (3000 g/m³, 45°C, 4 hours) was it possible to prove the formation of *N*-methyldaminoethanol; it was, however, not possible to prove the presence of ethylene glycol (24). Some 0.02 µg/ml of ethylene oxide were found in the smoke of guaranteed untreated cigarettes; fumigation increased this amount (25). No ethylene oxide residues were found in the tobacco 5 weeks after fumigation; the smoke, on the other hand, contained a higher ethylene oxide concentration even after several weeks (reaction with nicotine and reversion due to pyrolysis). Chlorohydrin was found in small quantities (12 µg/g) in the tobacco after fumigation; these rapidly disappeared under normal storage conditions and practically none was found in the smoke (0.5 µg/g). The smoke of untreated tobaccos already contained a small quantity of chlorohydrin (1 µg/g) (26).

Experiments concerning deactivation and the initiation of mutation of phagocyte Kappa of *Serratia marcescens* had the result that at least part of the damage could be attributed to DNS lesion. The humidity before and during fumigation had a decisive influence. The effects were first felt after several reaction stages with temperature-dependent rates (27). Whilst the classical sterilization processes (heat, steam) were based on momentary, irreversible physical reactions with proteins and nucleic acids, gas sterilization was a chemical reaction with the same cell components, which would, however, only take place under suitable conditions and after a longer period of treatment. A cell must contain sufficient moisture, if the gas molecule was to penetrate it. Vegetative cells usually fulfilled this requirement (without artificial drying), whilst spores dried out to a greater degree and were therefore more resistant. Not all alkylation products were lethal for the cell, which meant that ethylene oxide must be present in the cell in sufficient concentration to alkylize irreversibly certain essential groups. Increasing the concentration and raising the temperature, or moistening the goods, would not lead to successful sterilization; the only method was to ensure adequate conditioning. The use of bioindicators to determine the success of sterilization was only of any value if the method of preparing the indicator was adapted to the climatic conditions of the product and the indicator could be tested before use with the product. On the other hand, the preparations could also be manufactured in such a way that sterilization was absolutely impossible and their use as indicators thus became pointless.

The ethylene oxide-carbon dioxide mixture damaged some plastics (e.g., polystyrene). On the other hand, the mixture with methyl formate (ETOXIAT) did not (28, 29). Apart from drastically reducing the bacterial count, or even freeing the goods from bacteria, ETOXIAT could also reduce considerably the aflatoxin content. There was a direct relationship between the desorption of the physically-bonded ethylene oxide and the formation of ethylene chlorohydrin (33). Not only the values for the ethylene chlorohydrin residues

found by WESLEY *et al.* [*J. Food Sci.* **30**, 1037 (1965)] were too high, but those stated by HEUSER and SCUDAMORE [*Pest. Sci.* **2**, 80 (1971); *Pest. Sci.* **4**, 409 (1973); *Chem. Ind.* **16**, 1557 (1967); *J. Sci. Food Agric.* **20**, 566 (1969)] were also excessive because great quantities (up to 800 %) of ethylene chlorohydrin which were previously not present, were formed from ethylene oxide during the analysis through drying of the acetonic extract with sodium and calcium chlorides. On the other hand, the existent ethylene glycol was lost (34). Details of a better analytical method were to be published soon by K. PFEILSTICKER. No toxic effects from ethylene oxide-fumigated nutrition were observed in a two-year feeding test with rats: their appearance, behaviour, body weight, mortality, and organic structure remained unchanged, even with relatively high residues (initially: 500-1400 ppm; after 6 days: 53-400 ppm) (35).

Whilst hostaphan, rigid and plasticized PVC, and cellophane were in some cases considerably more permeable for ETOXIAT than for pure ethylene oxide, the differences in the cases of polyethylene, polypropylene, polyamide, and nitrocellulose were insignificant (36). Sorption in polyethylene, polyamides, silicones, aluminium membranes, and glass beads was noticeably slighter than in polypropylene, polystyrene, PVC, and paper. Desorption was more rapid in all cases if ETOXIAT was used in place of pure ethylene oxide (37-39).

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III. Phosphine

The chemistry of phosphine was no longer an unknown field. As its use increased in the stock protection sector, one found more and more publications in the appropriate literature.

Analytical methods were mostly based on the method proposed by WHITE and BUSHEY [*J. Amer. Chem. Soc.* **66**, 1666 (1944)] and were simply modified to meet the needs of the application in question (R.F. 1.1), e.g., they were also automated (R.F. 1.2). Residues in grain stock which, however, rapidly disappeared, could be determined with a sensitivity of 0.005 ppm (R.F. 1.3). By gas chromatographic methods, one could even determine 0.0005 ppm (R.F. 1.4, 1.15). A colorimetric method allowed sufficiently acute checking of the residue tolerances, even with smaller sample quantities (R.F. 1.11).

Analyses of fumigated grain, other foodstuffs, and animal feedstuffs, all revealed residues of 0.01 ppm or less. Vitamin analyses gave no indications of any changes (R.F. 1.5, 1.6). Metabolic analyses of fumigated grain also revealed no noticeable changes in the glutamic acid decarboxylase (R.F. 1.7), intensity of respiration, enzyme activity (R.F. 1.8). Differences just occurred at higher water contents of the grain, above about 18%. The differences up to about 20% were slight, then increasing rapidly, until a lethal effect on the seed was obtained at 25% (R.F. 1.9). The characteristic odour of the phosphine could already have disappeared whilst considerable quantities of gas were still present, because the very small odour-generating fractions were probably chemically bonded (R.F. 1.10).

In the case of phosphine, sorption of the gas in wheat or maize was practically insignificant. It just increased slightly with space utilization and higher moisture contents (R.F. 1.12). Quantities, added to grain products and inert materials could also be recovered in air-tight systems; losses only occurred at elevated temperatures in leaky systems. Chemisorption therefore did not

occur (R.F. 1.13). Even a 0.05 mm thick polyethylene film (R.F. 1.14) sufficed as a seal; those of polycarbonate, polypropylene, or cellophane were also practically impermeable, whilst kraft paper, even two-ply and resin-coated type, were moderately permeable (1).

Most of the toxicological questions connected with phosphine had also been investigated already. Publications which could be mentioned here as representatives were those of the Deutsche Kommission zur Prüfung gesundheitsschädlicher Arbeitsstoffe (2), the Belgian Répertoire des Pesticides (R.F. 2.1) and a German publication for the medical profession (R.F. 2.4).

Feeding experiments for 3 months with rats revealed no deleterious influences by the fumigated grain. Inhalation tests (8 hours) with house flies and grain weevils proved that the tablet residues also caused no toxication phenomena (R.F. 2.2). More extensive inhalation tests with cats, guinea pigs, and rats led to the finding that the application of 1 or 2.5 ppm of gaseous phosphine over more than 800 hours caused no cumulative toxification. The threshold concentration at which a subacute or lethal (depending on the duration of the application) toxification occurred, was probably about 5 ppm (R.F. 2.3). Chronic feeding studies over 2 years with rats that received a diet which had been fumigated at high concentration, also revealed no toxic effect (R.F. 2.5). In a suicide attempt, death was prevented by extracorporeal haemodialysis and medication with agents which supported the heart and circulatory system (3).

The effect of phosphine on insects was the theme of numerous publications. The resistance of insects differed, depending on their stage of development; e.g., the larvae of *Trogoderma sternale* were most difficult to destroy. With the c.t. products, it was found that a shortterm application of the gas was less effective than longer exposures (R.F. 3.1). In the case of 4 larger beetles, the egg stages showed the greatest resistance. With the exception of *Trogoderma sternale*, the adult insects were most susceptible, but even these showed greater tolerances than the adult lesser rice weevil, grain weevil, and confused flour beetle. One found no agreement between the tolerances of the individual stages of the different species (R.F. 3.4).

In the case of *Anthonomus grandis*, 9-10 day-old adults were less susceptible than 2-4 day-old (R.F. 3.5); in the case of various dried fruit pests, the eggs were the most difficult to destroy, whilst the larvae and adults were easy to eliminate (R.F. 3.6). The different stages of development of the grain beetle (*Sitophilus granarius*) showed increasing resistance: adult—larva—egg—pupa. But also within one stage there were differences, e.g., 1 month-old insects could already be eliminated with half the exposure time which was needed for freshly-emerged beetles (R.F. 3.7).

Fumigations with low concentrations (0.01-0.024 mg/l) led to the finding that the insect stages had developed further, and that viable eggs had even been laid. From this, one could conclude that the stages which were resistant at this concentration developed to less-resistant stages during the fumigation period and were then destroyed if the fumigation period was at least 10 days (R.F. 3.2). Sublethal fumigations when repeated, led to cumulative effects, different for each species. *Tribolium confusum* already recovered after 10 days, whilst *Sitophilus granarius* had not yet recovered after 40 days; *Tenebroides mauritanicus* behaved differently (4). The absorption of phosphine occurred only in the presence of oxygen. Without this, phosphine was not toxic, even when respiration failed, e.g., because of the effects of hydrocyanic acid or when the insects were previously treated with nitrogen or carbon dioxide. The

lethal action of phosphine did not increase with the concentration (applied in a scope of 5-20,000 ppm). High concentrations had a paralyzing action, similar to a narcotic effect, and decreased the respiration rate and thus also the mortality. Lower concentrations had a higher toxic effect on the insect: the increased amount of oxygen consumption might have accelerated the phosphine permeability in membranes of the cell and mitochondria. Then, phosphine would inhibit the respiration chain of the mitochondria, possibly cytochrome a_3 and b. On the other side, revival of insects at higher concentrations might be due to paralysis and reduced oxygen consumption, and it was likely that phosphine did not reach the toxic site of the cell. About 24 hours after treatment with 10,000 ppm, 50% of the insects were active, and the death of about 90% within 10 days indicated that they had absorbed a lethal dose of phosphine in a very short time before they became paralyzed. The last 10% of the insects (exposed to 10,000 ppm for 12 hours) survived for a period of 1 month and more, behaving normally as far as activity and reproduction were concerned. It was also possible that phosphine might be converted in the insect to nontoxic compounds, e.g., orthophosphate, as ROBINSON and BOND [J. Stored Prod. Res. 6, 133 (1970)] had found oxyacids of phosphorus within the tissues of insects. KLIMMER (R.F. 2.3) indicated the possibility of detoxification and excretion of phosphine in inhalation tests with warm blooded animals, too (7).

Cockroaches went into irreversible spasms after fumigation, the degree depending apparently on the concentration. The absorption differed with the species of insect; in no case was desorption observed (R.F. 3.3). In laboratory experiments with *Sitophilus granarius*, a triple tolerance was selected after 28 selection processes; this decreased somewhat after nine untreated generations, but stabilized once more after three further treated generations (5). *Spodoptera littoralis* had particularly resistant eggs; if these were, however, preconditioned for 3 days, their tolerance became equal to that of the larvae (6).

A summary by the American National Pest Control Association containing notes on the physical properties, application methods, insecticide properties, toxic effects, warning posters, and dosage recommendations, emphasized the international importance of the agent PHOSTOXIN (R.F. 4.1).

With various types of grain, pulses, and seeds, fumigation was found to have harmed the germination capacity in no way; indeed, it was thought to have improved it (R.F. 5.1-5.4). The effectiveness of phosphine as a fumigant for the control of pests in several fields of application had been studied. Sacked rice had been fumigated under gas-tight sheets (R.F. 6.2) and the lack of effect of the fumigation on organoleptic quality had been reported (R.F. 6.3). Natural raisins had been treated under craft paper, even repeatedly (R.F. 6.27). The fumigation of ground nuts (R.F. 6.7, 6.9, 6.10, 6.12, 6.30) was as successful as the treatment of soybeans (R.F. 6.35); there were no effects on the germination of seeds. Farinaceous products and processed commodities had been freed from insects (R.F. 6.14, 6.18, 6.26, 6.36).

A specially designed cocoa warehouse, which was however not gas-tight, had been treated with phosphine with good results and no injuries (R.F. 6.5, 6.8, 6.11, 6.25, 6.34). Good results had also been reported in connexion with the fumigation of sacked milho (R.F. 6.13).

Tobacco was fumigated with phosphine in several different packages, in warehouses, and in containers during transit, and the fate of the residues had been determined (R.F. 6.1, 6.19, 6.20, 6.21, 6.22, 6.23, 6.24, 6.31, 6.32, 6.33) (8). Successful studies were carried out in empty railway freight cars and in cars carrying bagged ground nuts, barley, and other grains and processed

cereal products (R.F. 6.15, 6.16, 6.29). Also reported upon was the fumigation of a mill with phosphine (R.F. 6.17).

Not only the common stored product pests could be controlled with phosphine. The pink bollworm (*Pectinophora gossypiella*) (R.F. 6.4, 6.28) had been controlled, and a method of controlling termites living within tea plants (R.F. 6.6) had been published.

In all parts of the world, scientists and practitioners were working with phosphine, publishing the results of their work and condensed reports in the relevant journals and magazines. A small selection had been made here from the great volume of literature.

From the European countries, the papers came from Belgium (R.F. 7.1.1), UK (R.F. 7.1.2), Yugoslavia (R.F. 7.1.3, 7.1.4, 7.1.6), and France (R.F. 7.1.5), whilst a further paper from UK dealt with the specific problems met in the tropics (R.F. 7.1.7). USA was represented with reports from home (R.F. 7.2.1, 7.2.2, 7.2.4) and overseas (Lebanon: R.F. 7.2.3) agricultural stations. Other papers came from Canada (R.F. 2.5, 7.2.6) and from Brazil (R.F. 7.2.7). Whilst further papers had been mentioned before (R.F. 6.7-12, 6.25, 6.34), some additional papers from the active Nigerian Stored Products Research Institute (R.F. 7.3.1-5) were added here. Asia participated in this series of publications with contributions from Japan (R.F. 7.4.1), India (R.F. 7.4.2, 7.4.5), and Turkey (R.F. 7.4.6).

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Appendix VII: Terminal Residues of Dithiocarbamates

Dithiocarbamates, especially the group of ethylene bisdithiocarbamates (EBDCs) were still the most extensively worldwide used organic fungicides. Since the last report given by KEARNEY (*Comptes Rendus XXVII Conference: Part B*, p. 256), there had been published some studies concerning the metabolic fate of EBDCs, particularly the formation and behaviour of ethylene thiourea (ETU), but only a few data about terminal residues of these compounds had been reported.

Metabolism

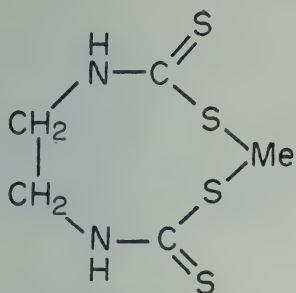
In Soil. HYLIN (1) had investigated the oxidative decomposition of nabam and maneb in soil as well as in solution and suspension, respectively. He proposed the following mechanism for breakdown of EBDCs:



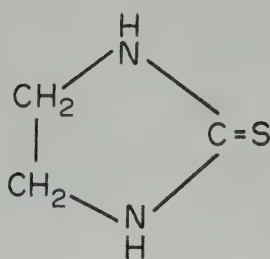
The behaviour of ETU in soils was studied by LYMAN and LACOSTE (2). ETU was found to be highly susceptible to photo and microbial degradation (formation of carbon dioxide) and consequently did not accumulate in soil. Soil tube leaching studies carried out with metiram had shown (3) that the active ingredient was strongly adsorbed in soils. No leaching could be observed with three different soils and amounts of rain as high as 200 mm applied within 48 hours.

In Plants. SIJPESTEJN and VONK (4) investigated the metabolism of nabam using the ^{14}C -labelled compound. After root as well as leaf treatment of cucumber, ETU, EU, and 2-imidazoline had been found in the plant plus a fair quantity of material not yet identified. ETU disappeared within 19 days and was almost quantitatively converted in the plant into 2-imidazoline and EU. DIDT, a spontaneous transformation product of nabam in aqueous solution, was not taken up by the plant.

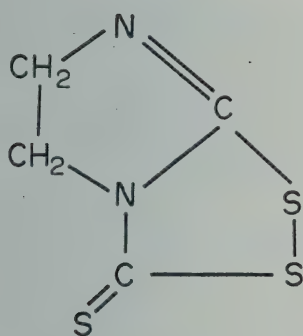
The effect of boiling on the formation of ETU in zineb-treated carrots, spinach, and tomatoes, was studied by NEWSOME and LAVER (5). From the data obtained it was evident that cooking promoted decomposition of the parent compound to ETU. Much of the ETU formed was removed in the cooking water but, compared to the uncooked samples, increased amounts remained in the crop. ENGST and SCHNAAK (6) reported about corresponding model tests with maneb-containing fruits. According to these authors, during



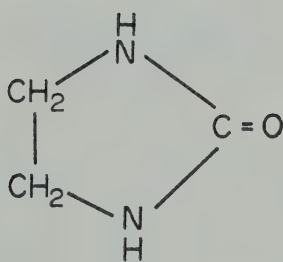
EBDC



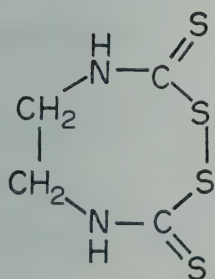
ETU



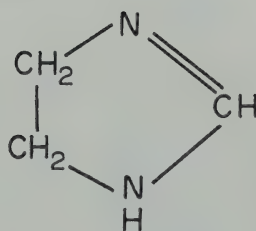
DIDT, EBIS



EU



ETD



2-Imidazoline

the thermal treatment the ETU residues could rise up to a tenfold amount compared with the starting material.

VOGELER and coworkers (7) reported preliminary results of experiments with ^{14}C -labelled propineb on apples and grapes under practical conditions. Relatively large amounts of the applied radioactivity were found in the peel and pulp of apples and in the juice and solid material of grapes. From the results obtained it was concluded that metabolism of propineb began with the parent compound being split into oligomeric fractions which were similar to the parent compound. According to LYMAN and LACOSTE (2) there was negligible uptake of ETU from soil and no significant translocation of ETU from leaf surfaces.

Residues

In Soil. KUHR and coworkers (8) analyzed soil samples from an apple orchard, which had been treated four times with metiram (total amount of active ingredient: 20 lb/acre). During the spray period, metiram residues accumulated in the top 2-inch soil layer up to a maximum of 6 ppm. For the following 4 months, residues, mostly below 1 ppm, were occasionally detected in the upper soil layer. No metiram was found in soil lower than 2 inches from the surface.

In Plants. NEWSOME (9) found ETU residues ranging from 0.02 to 0.04 ppm in commercial apple samples.

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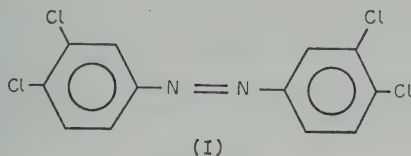
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Appendix VIII: Terminal Residues of Phenylamide-type Pesticides

Numerous phenylamide-type pesticides (phenylcarbamates, anilides, phenylureas, formamidines, *etc.*) had been shown to be hydrolysed to the corresponding anilines under certain laboratory and field conditions (1). In many of these studies the means used to establish the identity of the anilines and their rate of formation had clearly been deficient. However, in spite of lack of reliable and sufficient data, these preliminary observations provoked a host of experiments dealing with the further fate of substituted anilines in various biological media.

In 1967, BARTHA and PRAMER (2) reported that on application of high concentrations (500 ppm) of propanil [*N*-(3,4-dichlorophenyl)-propionamide] to soil samples, the herbicide decomposed to carbon dioxide and 3,4-dichloro-

aniline. The latter compound was condensed to form 3,3',4,4'-tetrachloroazobenzene (I). Soil microorganisms were demonstrated to be involved in both transformation reactions.



Formation of symmetrical azobenzenes was subsequently shown to occur with or from high concentrations of phenylcarbamates, anilides, formamides, and free, substituted anilines in a variety of different model systems, including soil suspensions, microbial cultures and photolytic media (3). In addition, further condensation products, such as asymmetrical (hybrid or mixed) azobenzenes, azoxybenzenes, anilinoazobenzenes, triazenes, *etc.*, were demonstrated to be formed, depending on the concentrations of the anilines, the position of their substituents, and the conditions chosen for the experiments (4-6). To elucidate the potential pathways of formation of the mentioned condensation products, a number of studies were conducted, both with biological (including enzymatic) and chemical (sensitized-photosensitized) systems. These experiments indicated that the intermediates to be observed were dependent on the relative concentrations of the various potential reactants. However, most of the proposed transformation mechanisms involved one or more oxidative steps and the formation of radicals (5).

Although the various laboratory and model experiments were normally carried out with concentrations of anilines and aniline-containing parent compounds far beyond those applied or detected in practice, conclusions were drawn in many papers and even in press releases with regard to the environmental significance of condensation products derived from phenylamide pesticides. In regulatory terms, these implications were amplified by illusions made to toxicological effects of certain azobenzene derivatives (7, 8). Meanwhile, a number of experiments had been conducted in which the concentration of phenylamide pesticides and free aromatic amines approached those to be expected in practice. Those studies were facilitated by the high sensitivity of gas chromatographic methods, by which condensation products of anilines, especially halogenated azobenzenes, could be determined (9, 10).

Free 3,4-dichloroaniline was applied by SPOTT and CORKE (6) to four different Canadian soils. Even at the relatively high concentration of 100 $\mu\text{g/g}$ soil (100 ppm), the conversion to 3,3',4,4'-tetrachloroazobenzene was minimal (0.0-0.6% in terms of applied 3,4-dichloroaniline). These data, which indicated that the formation of condensation products was strongly dependent on the concentrations of anilines and was significantly reduced or nonexistent at their practical levels, was confirmed by several studies (11-14).

Extensive investigations with phenylureas, both in the laboratory and under field conditions, demonstrated that no detectable amounts of condensation products, such as azobenzenes, were generated from these herbicides in soils or plants (9, 10, 15, 17). Apparently, the rate of formation of free anilines from phenylureas was too small to allow sufficient buildup for condensation reactions. The same situation applied to formamides (18). A recent report from the Pesticide Monitoring Laboratory Bay at St. Louis, Miss., showed

that from among 99 different soil samples derived from rice fields treated with propanil for 1 to several years, only 6 were found to contain traces of residues of 3,3',4,4'-tetrachloroazobenzene (0.01-0.05 ppm).

From present evidence it was concluded that the condensation products discussed above did not represent significant terminal residues of anilides, phenylcarbamates, phenylureas, and formamidines in agricultural soils. From recent reports in the literature (12-14) it appeared that certain binding or conjugation reactions with soil constituents were more important for aniline-containing pesticides. These reactions deserved further attention.

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Appendix IX: Fate of Chlormequat in Wheat Plants

Fate of Chlormequat in Wheat Plants. One of the major problems that confronted both regulatory agencies and the pesticide industries was how to recommend maximum tolerable amounts of the pesticide itself and its transformation products. In practice, one had to rely on data which were collected from different sources. Conflicting data had been reported, due to the use of different analytical procedures or in the form in which a compound was applied to a plant. The pattern of transformation products obtained and especially the rate of disappearance of the parent compound and its transformation products might depend on the way the compound had been applied to the plant.

The work of DEKHUIZEN *et al.* on chlormequat showed that the compound when taken up by the roots of wheat seedlings (for 6 hours) was rapidly translocated to the above ground parts and converted to choline. Choline was further metabolized to betaine, which on demethylation yielded finally glycine, serine, and $^{14}\text{CO}_2$ [DEKHUIZEN and VONK (1974); DEKHUIZEN

(1974)]. 50% of the total amount of chlormequat originally present in whole wheat seedlings was already metabolized after 7.5 days. This result was most consistent with results reported by MOONEY and PASARELA (1967) and by JUNG and EL-FOULY (1966) after spraying chlormequat on wheat plants. However, the results were not in agreement with those of BIRECKA (1967) and BOHRING (1972, 1974), showing no decrease of chlormequat after root or leaf application over a 4-week period.

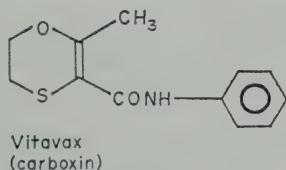
These discrepancies were difficult to explain and might be due to the use of different wheat varieties or different environmental conditions during the experimental period. Another explanation might be that chlormequat was taken up more slowly by the leaves than by the roots and consequently a deposit remained for a long time on top of the leaves [see also BLINN (1967)].

Effect of Site of Application on Metabolism. The problem of the rate of disappearance of chlormequat raised several general questions. For the chemical identification of a terminal residue it was often a necessity to raise the amount of the applied compound as high as possible. For that purpose it was possible to use root application, stem injection, or uptake into an excised leaf via the cut end of the petiole. However, this did not tell one anything about the rate of disappearance under practical conditions. To obtain quantitative information on the rate of disappearance of the parent compound and various transformation products, it could be recommended to use a method of treatment of the plant (leaf application in the case of most herbicides and growth regulators) which paralleled as closely as possible the actual field application.

A further point which was often neglected in this context was the fact that metabolism of a pesticide was dependent on the (physiological) age of plants, at least in quantitative terms. Thus, the terminal residue situation in mature plants (e.g., grain and straw) was normally quite different from that found in young, immature seedlings.

Although the above matters were well known to laboratories which dealt regularly with Regulatory Authorities (especially in USA), they were often not considered or recognized in publications on pesticide metabolism.

Aniline Formation from Various Types of Pesticide. According to GEISSBÜHLER (1971) and to FREAR and SWANSON (1972), degradation of urea herbicide to the corresponding anilines did not represent a major pathway of transformation in animals and plants. Aniline derivative formation seemed to be more important in soils, although a detailed balance of radioactivity derived from ring labelled ureas was lacking. This became more urgently needed, because of the use of aniline-containing fungicides for seed treatment (oxathiins).



Carboxin was rapidly oxidized. Hydrolysis in water of soil did not take place [CHIN (1971)]. However, this was in contrast with results obtained by BOCHOFFER (1973). Soil bacteria of the species *Nocardia* (enrichment, culture) were able to grow on a medium supplemented with carboxin or aniline as a sole carbon and nitrogen source.

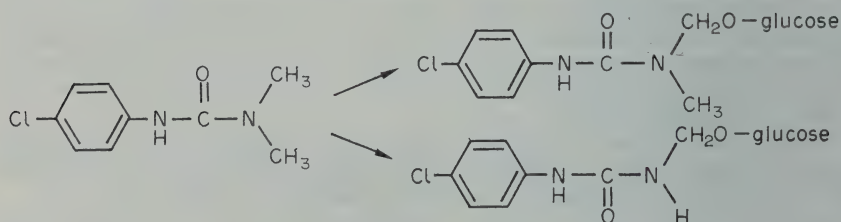
Recently, McCLURE (1974) demonstrated that microorganisms grew and respired rapidly on nonchlorinated aniline herbicides, but ring chlorination depressed respiration and inhibited growth. Hydrolysis of the side chain (yielding the corresponding aniline derivative), followed by metabolic degradation of the phenyl ring, could be shown in a number of cases.

In light of these results it could be recommended to urge a more detailed study on the fate of aniline-containing pesticides in soil and an elucidation of the pathway for the breakdown by microorganisms.

Complex Formation of Aniline-containing Pesticides

Complex Formation with Lignins. SHEL and EDGINGTON (1970) and CHIN *et al.* (1970) found complex formation between carboxin and plant lignins. It still remained an open question whether the whole molecule was involved in complex formation or whether aniline was first produced, then bound to polymers. According to GEISSBÜHLER (pers. comm.) free anilines might be bound to certain lignin-type or humic acid-type constituents as had been demonstrated by several people. However, nobody had shown that this applied to phenylurea-derived anilines.

Glycoside Complex Formation. As far as ureas were concerned, there was definite evidence from the work of FREAR and SWANSON (1972) and of LEE and FANG (1973) that monuron formed a glucoside in plants. However, it was *not* the free aniline which was conjugated, but the parent compound or its demethylated and/or hydroxylated derivatives.



Ring hydroxylation followed by glucosidation had been shown by LEE and FANG (1973). On the other hand, the results showed a monuron polypeptide complex formation. Further studies on complex formation of aniline containing pesticides might be recommended.

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Appendix X: Photodecomposition of Chlorinated Pesticides

Previous reviews had included the photochemistry of chlorinated insecticides (1), chlorinated herbicides (2), the fate of such compounds in the atmosphere (3), and their transformation by photosensitized processes (4). The photochemistry of cyclodiene insecticides, reviewed in part by Benson (5), were covered in Appendix I (p. 23).

Chlorinated Aliphatic Hydrocarbons. Many simple chloroalkanes received wide use as fumigants— CHCl_3 , CCl_4 , Cl_3CCH_3 , and $\text{ClCH}_2\text{CH}_2\text{Cl}$, for example. However, they did not absorb light at wavelengths above 290 nm, the sunlight region of the spectrum at the earth's surface (6). While radical reactions could be expected to occur in the upper stratosphere (above about 40 km) where the necessary radiant energy was available (7), their association with 'terminal residue' concerns was presently speculative.

Both as vapour (8) and liquid (9), 1,1,2,2-tetrachloroethylene (perchloroethylene) was photooxidized to its epoxide, followed by rearrangement to trichloroacetyl chloride or (in the presence of water) trichloroacetic acid. 1,1,2-Trichloroethylene behaved similarly (10), producing dichloroacetyl chloride, trichloroacetaldehyde, and phosgene. The use of these chlorinated hydrocarbons as space fumigants probably precluded photoproducts as terminal residues in food, but their annual billion-pound use as cleaning solvents almost certainly resulted in atmospheric transformation to gaseous products. The closely related soil fumigants telone and D-D mixture (isomeric 1,3-dichloropropenes) appeared to be unreactive at sunlight wavelengths (11).

Chlorinated Aromatic Compounds. Pentachlorobenzyl alcohol, a rice fungicide, was rapidly degraded under UV irradiation in aqueous methanol (12), probably to the corresponding aldehyde and acid in analogy to the mono-, di-, and trichlorobenzyl alcohols (13). The simultaneous formation of a large proportion of ionic chloride was also consistent with the replacement of Cl by H and OH observed with the less-chlorinated analogues as well as many other aromatic halides (14). Composition of the terminal residue would depend primarily on the absorbance of the resulting isomeric chlorobenzoic acids in the sunlight region and the subsequent reduction and hydroxylation (14a).

DDT had long been known to decompose in sunlight or laboratory UV light (15). The initial products from homolysis of the aliphatic C-Cl bond, DDD and DDE, were prominent products of most DDT photolysis. With filtered mercury arc light, DDT in methanol formed a variety of oxidation products (detected only by mass spectrum) (16), and these and other substances also were formed by UV irradiation of DDT or DDE in water (17). Photodecomposition was slow in sunlight, but sensitization allowed extensive breakdown to oxygenated products, including DDA, dichlorobenzophenone

(DCB), and *p*-chlorobenzoic acid within 24 hrs. These products could be explained by formation of a (still hypothetical) intermediate, DDT epoxide (Fig. 1) (17). DDMU was also commonly observed.

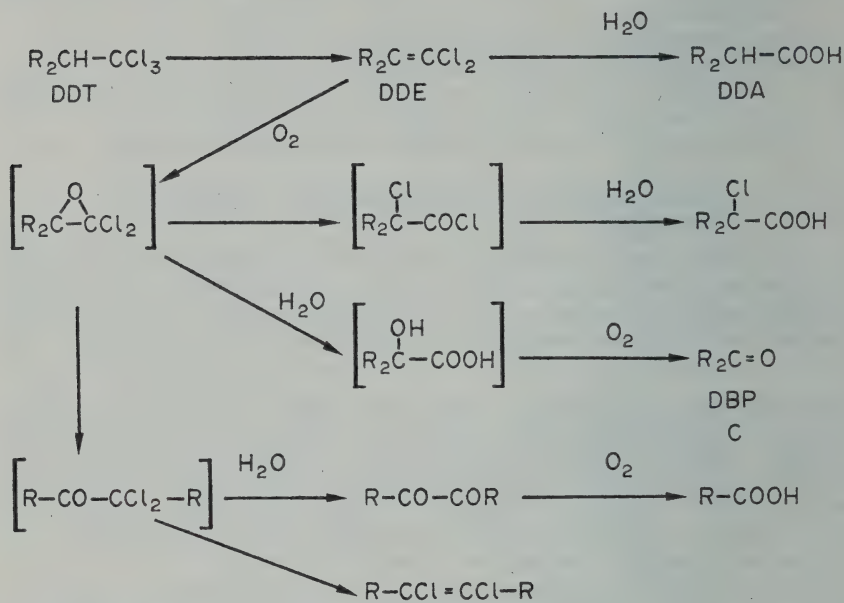


Fig. 1. R = *p*-chlorophenyl

A number of natural and synthetic substances acted as photosensitizers for DDT (18), although DDE and DCB were the only products detected from sensitized photolysis on leaf surfaces (19). However, irradiation of unsensitized DDT or DDE as vapour showed surprisingly facile dehydrochlorination, oxidation, and fragmentation to provide lower members of the chlorobiphenyl series (PCBs) (20). 2,7-Dichlorofluorenone, readily formed from crystalline DDE in sunlight (21), had not been isolated under other circumstances, but a 'DDE isomer' probably containing three chlorines on the aromatic rings was detected (along with the usual products) from irradiation of DDE as a solid, in solution, and in the vapour phase (22).

Methoxychlor solutions were easily photolyzed in sunlight to yield the DDE-DCB analogues as well as *p*-methoxybenzoic acid and *p*-methoxyphenol (23, 24). Therefore, terminal photolysis products from other insecticides of the DDT series might be expected to include the olefin, ketone, and acids; the environmental presence of these compounds had been verified in field experiments with DDT (25, 26). The methoxychlor analogue MPA [1,1,1-trichloro-2,2-bis(5'-chloro-2'-methoxyphenyl) ethane] decomposed at sunlight wavelengths to give the expected products (27), and its olefin absorbed strongly in the sunlight region to give primarily 2,5-chloro-3-(5'-chloro-2'-methoxyphenyl)benzofuran (28).

Chlorinated Aromatic Hydrocarbons. Although irradiation of a methanolic solution of hexachlorobenzene, the major impurity in dacthal herbicide, resulted only in isolation of an antifact, pentachlorobenzyl alcohol (see above)

(29), the facile photoreduction of pentachlorobenzene and isomeric tetrachlorobenzenes to less-chlorinated homologues in organic solvents would be expected to apply (30).

The polychlorinated biphenyls also underwent photoreduction on irradiation with sunlight or UV light under a variety of conditions (31-35). In solution or suspension, oxidation, replacement of Cl by OH, and polymerization to complex products were also observed (32-36), although pure PCB isomers were stable as vapour (20). The hydroxylated derivatives were as toxic to insects as common insecticides, such as aldrin (36). Considering the alleged stability of PCBs, these results were surprising; an acute toxic hazard from PCB photoproducts possibly could exist, interpretation of a PCB terminal residue to represent any particular commercial product (such as Arochlor 1254) might well be erroneous, and the lower PCBs were probably terminal products of DDT photolysis only as long as they remained in the atmosphere.

Other Chlorinated Pesticides. A sizable proportion of the common pesticides contained chlorine, so a complete review obviously lay outside the scope of the present discussion. However, several examples which illustrated reactions of the C-Cl bond were particularly pertinent to the question of photochemical terminal residues. The phenoxy herbicides, such as 4-CPA (37), were photodecomposed in water at sunlight wavelengths by common processes of sidechain oxidation and the usual replacement of the halogen by hydroxyl and by hydrogen (Fig. 2).

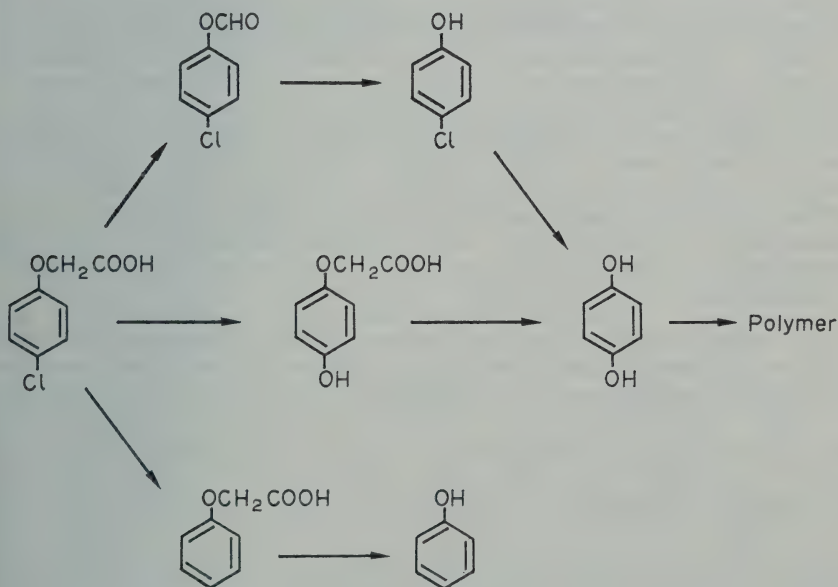


Fig. 2

The photooxidation was readily sensitized, causing appreciable conversion of 2,4,5-T to the corresponding phenol within a few hours (38). Pentachlorophenol (PCP) solutions underwent analogous photoreduction and hydroxyla-

tion (39, 40), followed in the latter case by oxidation to chloranil, chloranilic acid, and further products of both condensation and rearrangement (Fig. 3).

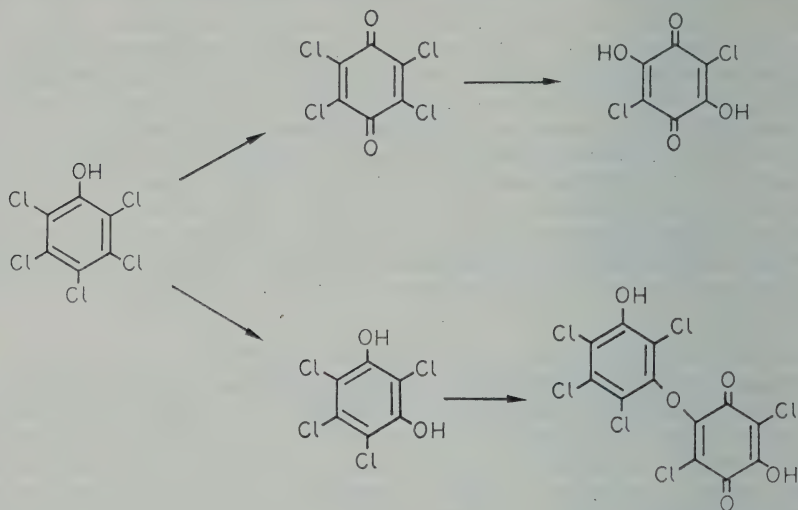


Fig. 3

The photonucleophilic generation of phenols with hydroxide ion (14) suggested that *o*-chlorophenols might condense to form chlorinated dibenzo-*p*-dioxins. While this transformation had been demonstrated with solutions of sodium pentachlorophenate (NaPCP) (41), the dioxins themselves were so readily dechlorinated and cleaved in light (42) that lower chlorinated members of the series—such as tetrachlorodibenzo-*p*-dioxin (TCDD)—could not be detected. Replacement of the *m*-chlorine of PCP by hydroxyl provided relatively stable tetrachlororesorcinol, while the corresponding tetrachlorohydroquinone and tetrachlorocatechol formed a stable chlorocyclopentanedione (43). Displacement of the aromatic nitro substituent in PCNB (pentachloronitrobenzene) to give tri- and tetrachlorobenzenes, accompanied the displacement of chlorine (40).

Environmental Photochemistry and Terminal Residues. At present, the exact relation of photochemical processes to pesticide dissipation and terminal residues remained unknown. While pesticide photodecomposition by sunlight was often demonstrable under idealized conditions, classical photochemistry generally had not provided predictability for real environments. This was due largely to the dependence of photolysis pathways on the immediate chemical environment of the pesticide. The previous examples revealed the action of both radical reagents (oxygen and organically-bound hydrogen) and ionic ones (hydroxide ion and other nucleophiles), often working in concert as with 4-CPA. While laboratory experiments allowed the formulation of general mechanisms, accurate knowledge and recognition of the natural micro-environments were usually lacking. For example, the toxic dioxin impurities of 2, 4, 5-T were rapidly photoreduced *in vitro* to harmless products in the presence of organic solvents but otherwise appeared quite stable (*e.g.*, as a crystalline solid) (40). But in what form did the dioxin actually exist on the sprayed surface of a leaf—as stable solid, or dispersed in cuticular leaf wax,

or still dissolved in the mixture of hydrogen-donating solvent and pesticide in which it was inadvertently applied?

The chemical nature of the formulation, then, was of immediate importance to pesticide photodecomposition and its terminal residues. The hydrocarbon solvents used in emulsifiable concentrates provided hydrogen atoms for photoreductions (44). Dust particles (usually represented by silicic acid in the laboratory) provided sites which could cause significant changes in both the reactivity and light absorption of adsorbed pesticides (1). Photosensitization, often by common natural products, such as chlorophyll or riboflavin, occurred in both aqueous and organic solution as well as on leaf surfaces (4). And photochemical reactions in organic surface films and micelles stabilized by surfactants often occurred at greatly accelerated rates (45).

The ability of the C-Cl bond to undergo homolytic cleavage in light, as well as photonucleophilic displacement of chloride ion by nucleophiles, caused chlorinated pesticides to be exceptionally reactive. However, terminal residues might actually be dictated by light absorption; e.g., PCB isomers were photoreduced only down to the stable monochlorobiphenyl which no longer absorbed in the sunlight region (32). Terminal residues might also be dictated by subsequent nonphotochemical processes; photooxidation and photonucleophilic hydroxylation of 2,4-D eventually formed 1,2,4-benzenetriol, which underwent rapid air oxidation to polymeric humic acids even in the dark (46).

The identity of photolysis products with products of metabolism—in DDT, for example—compounded the confusion over the significance of photodecomposition to terminal residues (47). However, the current surge of interest in environmental photochemistry promised eventual clarification of many of these important issues.

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COMMISSION ON PESTICIDE RESIDUE ANALYSIS (VI.5.2)

Bracknell, 3 October 1974

Present: Dr. H. FREHSE (Chairman), Dr. P. SLADE (Secretary), Dr. D. C. ABBOTT, Dr. V. BÁTORA, Dr. K. R. HILL, Prof. P. E. KOIVISTOINEN, Dr. P. B. POLEN, Prof. G. WIDMARK (Titular Members); Mr. K. E. ELGAR, Dr. S. GORBACH, Dr. CH. RESNICK (Associate Members); Dr. H. M. DEKHUIJZEN, Dr. S. DORMAL VAN DEN BRUEL, Dr. N. DRESCHER, Mr. M. J. EDWARDS, Prof. R. ENGST, Dr. H. GEISSBÜHLER, Dr. R. GREENHALGH, Dr. P. A. GREVE, Dr. J. MIYAMOTO, Mr. A. J. PIETERS, Dr. P. E. PORTER, Dr. E. E. TURTLE (Observers).

1. Minutes of Previous Meeting

The minutes of the Seventh Meeting of the Commission, held in Munich on 25 August 1973, had been published, together with Appendices, in *Comptes Rendus XXVII Conference, Part B* (see pp. 303-326). Item 4 (iv) should be amended to read in the first sentence '... for each pesticide in each substrate.'

2. Matters Arising from Minutes

- (i) *Minute 4* (i). Dr. FREHSE reiterated that the Commission would welcome the attendance at its meetings of analysts from developing countries. Dr. TURTLE agreed that such delegates should attend when convenient.
- (ii) *Minute 5*. The Secretary again requested that reports should be accompanied by a summary. They should also be written in IUPAC-approved style.

3. Membership

Dr. SLADE had to relinquish the post of Secretary because of pressure of work. Prof. KOIVISTOINEN was nominated as his successor.

4. International Liaison (see also p. 18)

- (i) *CEE*. Dr. FREHSE asked if it was possible for CEE to draw the Commission's attention to its requirements for analytical methods. Dr. DORMAL VAN DEN BRUEL agreed to do this.
- (ii) *COMECON*. Prof. KOIVISTOINEN suggested that an official delegate representing the residue analytical interests of COMECON should be invited to the next meeting. This was agreed.
- (iii) *FAO-WHO*. The requirements for analytical methods emerging from the 1973 FAO-WHO JMPR involved the following compounds: benomyl, carbaryl, tricyclohexyltin hydroxide.
- (iv) *CCPR*. A list sent to Dr. FREHSE by Dr. GREVE in May 1974 indicated analytical method requirements from CCPR for: binapacryl, captafol, captan, crufomate, dichlorvos, dioxathion, ethion, ethoxyquin, folpet, HCB, hydrogen phosphide, lindane, malathion, *o*-phenylphenol, parathion, phosphamidon, pyrethrins, quintozone, thiabendazole.

5. IUPAC Technical Reports

Some progress had been made during the year in preparation of the Commission's recommendations on analytical methods for publication as an IUPAC Technical Report. Mr. ELGAR and Mr. HEUSER submitted draft

documents on the analysis of organochlorine insecticides and of fumigants. It was agreed that revised versions of these documents and similar summaries of recommendations for analysis of other compounds, would be circulated to Commission Members prior to the next meeting when final versions would be prepared.

6. Organochlorine Compounds

Mr. ELGAR reported (see Appendix I) on recent work on the multiresidue method recommended by the Commission in 1969. Studies had included a comparison with other multiresidue methods, extraction from soil and from blood, and a rapid method for milk. There had been important progress during the year towards solving the problem of the separation and estimation of the PCBs. Perchlorination with antimony pentachloride gave the decachlorobiphenyl, which was separated from the organochlorine insecticides. Other studies had included work on cleanup adsorbents, on the electrolytic conductivity detector, and on analysis of the polychlorinated dioxins. Dr. GREENHALGH pointed out difficulties in the use of the antimony pentachloride for PCBs. Dr. BÁTORA drew attention to two papers describing the determination of BHC isomers in soil and water [J. UHNAK *et al.*, *J. Chromatog.* **89**, 177 (1974); H. MAHEL'OVA *et al.*, *ibid.*, **91**, 545 (1974)].

7. Organophosphorus Compounds

Dr. FREHSE presented a paper (Appendix II) describing recent advances in residue analytical methodology for organophosphorus compounds. He selected five analytical procedures for multiresidue determinations and indicated to which compounds each method could be applied. Also, he discussed methods applicable to chlorpyrifos, coumaphos, crufomate, demeton, fenamiphos, fensulfothion, methidathion, monocrotophos, trichloronat. Mr. EDWARDS stated that a method for pirimiphos methyl and its metabolites in crops was shortly to be published [*Analytical Methods for Pesticides and Plant Growth Regulators*, G. ZWEIG (Ed.), Academic Press, in press].

Dr. BÁTORA presented a paper (Appendix III) on methods reported recently in COMECON countries. Thin layer chromatography (tlc) using enzymatic and/or chemical detection seemed to be the predominant technique for routine screening and estimation of organophosphorus residues. Column separation of parent organophosphorus compounds and metabolites and modified sweep codistillation cleanup was suitable for multiresidue analysis. A simple alkylation technique followed by gas liquid chromatography (glc) was suitable for chemical confirmation at the submicrogram level.

There was a discussion, initiated by some comments in Dr. FREHSE's paper, on the Commission's philosophy on the principles governing the recommendation of residue analytical procedures and multiresidue methods for metabolites. Dr. GEISSBÜHLER felt that multiresidue methods were not usually suitable for metabolites; if the parent compound was present, it was necessary to look separately for metabolites. Dr. ABBOTT said that in his experience, organophosphorus compounds were seldom observed in food samples, other than cereals, so that it was not often necessary to seek metabolites. Dr. ABBOTT stressed that if residues appeared to exceed the tolerance level, it was essential to apply confirmatory methods. Dr. GREVE said that he had found tlc methods were useful as confirmatory tests, although Dr. FREHSE considered no recommendation was possible for any specific tlc method.

Dr. DORMAL and Dr. ABBOTT referred to methods for analysis of organo-phosphorus compounds under discussion in CEE, including an unpublished method evolved by the National Food Institute in Denmark. Collaborative studies were underway to validate these methods. Dr. FREHSE's paper could be useful in the CEE discussions.

Mr. PIETERS asked whether different results were obtained when different methods were used. Dr. ABBOTT stressed that the really important factor was that any method should be validated in the worker's own laboratory. Differences were more likely to arise from sampling problems than the analytical methods themselves.

8. Carbamate Compounds

(i) *Insecticidal carbamates*. Dr. ABBOTT presented a paper (Appendix IV) on this subject. In the last year methods had been developed for the determination of residues of carbaryl, promacyl, mesurol, carbofuran, aldicarb, and methomyl, in a wide range of substrates. The formation of electron-capturing derivatives for glc continued to be the most favoured technique for both single and multiple carbamate residue determinations. For multiresidues the successful application of fluorogenic labelling combined with liquid chromatography had been reported.

Dr. HILL explained that the results of a collaborative study in USA of the method involving the glc of 1-fluoro-2,4-dinitrobenzene derivatives were to be reported shortly. Mr. EDWARDS drew attention to the fact that pirimicarb and two of its metabolites could be analyzed by glc using a nitrogen detector [*Analytical Methods for Pesticides and Plant Growth Regulators*, G. ZWEIG (Ed.), Academic Press, 7, 399 (1973)].

Dr. FREHSE pointed out the need for a reliable analytical method for carbaryl (the 1973 FAO-WHO JMPR had requested a method for carbaryl in milk, but the problem was a general one). He also suggested that there was a need for collaboration with the Terminal Residues Commission to determine which residues needed to be measured. In this connexion Dr. HILL drew attention to the problems of hydroxyl-containing metabolites of carbamates. Requests were being made for analysis of these compounds.

(ii) *Herbicidal carbamates*. Dr. RESNICK presented a paper (Appendix V) on this subject. Direct glc of these compounds using a Coulson electrolytic conductivity detector might be developed for residues because a suitable cleanup procedure seemed to be available; work was required on devising a suitable combination. Dr. GREENHALGH commented that Coulson detectors were already used for analysis of herbicidal carbamates in Canada.

9. Fumigants

Mr. S. G. HEUSER had submitted a paper (Appendix VI) on developments in methods of analysis of residues from phosphine, methyl bromide, ethylene oxide, and other fumigants. Collaborative testing of a multiresidue method for chlorinated hydrocarbon and other fumigant residues between eight UK and Dutch laboratories had been successfully completed, and would be published in *The Analyst* during 1974 (99, 570). The group was now to conduct collaborative tests on a glc method for bromide ion in cereals.

Dr. CROSBY drew attention to a polarographic method for bromide residue determination [H. BECKMAN, P. T. ALLEN, D. G. CROSBY, W. O. GAUER and C. MOURER, *J. Food Sci.* 32, 595 (1967); *ibid.*, 32, 138 (1967)].

It was agreed that at next year's meeting of the Commission there should be a joint meeting with the IUPAC Food Section to discuss bromide analysis.

10. Systemic Fungicides

Dr. GORBACH presented a paper (Appendix VII) on the recent work in this field. Only a few new methods had been published. Mr. EDWARDS said that the residue analytical method for ethirimol using glc with a nitrogen detector following derivative formation was to be published shortly [*Analytical Methods for Pesticides and Plant Growth Regulators*, G. ZWEIG (Ed.), Academic Press, in press]. Dr. ABBOTT drew attention to a recent review of analytical methods for systemic fungicides [P. B. BAKER and R. A. HOODLESS, *Pestic. Sci.* 5, 465 (1974)]. Dr. RESNICK suggested that there might be an increasing need for analytical methods for metabolites of systemic fungicides.

11. Dithiocarbamate Fungicides

Dr. RESNICK presented a brief review (Appendix VIII) of recent work in analysis of dithiocarbamates, including a microbiological method. Prof. ENGST said that such methods required to have a cleanup procedure incorporated, and Dr. ABBOTT pointed out the difficulty of making them both specific and quantitative at the same time. The importance of ethylene thiourea (ETU) as a terminal residue was discussed. Dr. BÁTORA commented on its presence in technical dithiocarbamates. It was recommended that the FAO-WHO JMPR should give consideration to the possibility of assigning a specific residue limit to ETU, in view of its constant occurrence following crop treatments with the dithiocarbamate fungicides and its toxicological significance.

12. Tin Compounds

Prof. KOIVISTOINEN presented a manuscript of a paper which he had prepared for publication in *Residue Reviews*. The analysis of residues of tin compounds had proved difficult. Total tin could be measured, although it was unsuitable to measure tin derived from pesticides in view of the variable tin content of many foodstuffs.

Dr. TURTLE said that the 1970 FAO-WHO JMPR had asked for the establishment of analytical methods for determining separately cyclohexyltin and other organotin compounds. Such methods were not yet available, but recently described glc techniques might be capable of development into such a method. Dr. GORBACH said that at present a colorimetric method was capable of detecting tin down to 0.05 ppm.

13. Rethrins and Synergists

A short paper on rethrins and synergists was presented by Dr. HILL (Appendix IX).

14. Summary of Compounds Not Covered

Dr. FREHSE listed the compounds of interest to Codex but not covered by the reviews presented to the Commission. These were: binapacryl, captafol, captan, ethoxyquin, folpet, *o*-phenylphenol, quintozene. Arrangements were made for these to be kept under review by individual Members of the Commission.

15. Selective Detectors

Mr. EDWARDS introduced a paper from Dr. W. AUE (Appendix X) in the

latter's absence, and included some observations from his own experience. A copy of his views was circulated to Members.

16. Limits of Detection

Dr. GORBACH had begun to collect views from Members on this subject during the past year, and agreed to prepare a comprehensive paper summarizing their comments at the next meeting.

17. Next Meeting

It was agreed that if possible the next meeting should include a half-day working session on techniques and state-of-the-art, *etc.* Dr. GREENHALGH would prepare a paper on confirmatory tests, and Mr. ELGAR would prepare one on the statistical deviation of results. The meeting would take place during the 28th IUPAC Conference, in Madrid, in early September 1975.

P. SLADE

Appendix I: Multiresidue Methods of Analysis for Organochlorine Compounds

Further studies to expand and strengthen the multiresidue method for organochlorine residues (1) recommended by IUPAC continued to be made and this report reviewed the data published in the last year. Much of this progress was under the auspices of AOAC and the reports of the General Referees, J. A. BURKE on chlorinated pesticides (2) and P. A. CORNELIUSSEN on multiresidue methods (3) summarized their recent work.

General. Additional general studies included that by SMART *et al.* (4) who compared the AOAC, the DE FAUBERT MAUNDER (5), WOOD (6) and an unpublished CEE method. They concluded that there were no gross differences between results obtained with these methods, although for certain foodstuffs and in certain situations some methods appeared preferable to others. HOLDEN (7) had reported an international cooperative study with organochlorine residues by 26 laboratories in 12 countries. The analytical method was based on extraction, cleanup, and glc determination, but no two laboratories used exactly the same procedure. Nonetheless, there was reasonable agreement in the analysis of test samples with coefficients of variation for different organochlorines ranging from ± 10 to $\pm 17\%$.

Extraction. WOOLSON (8, 9) had reported two studies on the extraction of organochlorine compounds from soil. In the first, shake, Soxhlet, and column methods were compared, and in the second, soil premoistened with 0.2M ammonium chloride, then shaken with a hexane-acetone mixture (1:1), was studied collaboratively in 7 laboratories. Recovery of 6 organochlorines from spiked samples was 91% with a coefficient of variation of 13.5%.

Cleanup. CLAEYS and INMAN (10) had compared Florisil, alumina, and silicic acid, for their ability to retain lipids and found that a basic alumina retained more than Florisil, which in turn held more than silicic acid. Also, they found that deactivation and elution with less polar solvents gave a superior separation of organochlorines from lipids than activated adsorbents and more polar elution solvents.

Analysis and Confirmation of Residues. The multiresidue method had been extended to the analysis of whole blood (11). The method used sulfuric acid to free pesticides from the substrate. Analysis of the data from 11 collaborators

revealed a large systematic error and further studies were to be carried out. A rapid version of the multiresidue method for milk had been studied by GABICA *et al.* (12) and had been found useful for the screening of large numbers of samples.

The electrolytic conductivity detector as a possible alternative to the electron capture detector had been investigated by DOLAN and HALL (13) and they found that after modification the detector had a useable response to sub-nanogram amounts of a number of organochlorine insecticides. Optimization of several factors enabled the organochlorines to be determined in the presence of PCBs with a selectivity of the order 1000 to 1.

Chemical reactions that could give confirmation of residues continued to be studied, for instance, in the last year by COCHRANE and MAYBURY on BHC isomers (14) and by CHAU *et al.* on heptachlor (15).

Polychlorinated Biphenyls. The determination of organochlorine insecticides in the presence of PCB had now become an established procedure. The separation of the higher chlorinated members from DDE in particular had been carried out by column chromatography on silica gel (16) and had been incorporated into the general analytical schemes (17, 18). However, separations were not easy to achieve and investigations into column chromatography (19), oxidation of DDE to dichlorobenzophenone (20) and gas chromatography-mass spectrometry (21) had been published in the last year. A further procedure that assisted the analysis of residues of PCBs was the use of the perchlorination procedure published by BERG *et al.* (22) and further investigated by ARMOUR (23) and by HUCKINS *et al.* (24). The chlorination was carried out with antimony pentachloride to give a single derivative from all the members of the group, the fully chlorinated decachlorobiphenyl. The procedure increased the sensitivity of the determination and the ease of identification of the group. Care must be taken with the purity of the antimony pentachloride, traces of bromide leading to the production of monobromonachlorobiphenyl.

Polychlorinated Dibenzo-p-dioxins and Dibenzofurans. A review of the USDA studies on the sources, analysis, and environmental monitoring of these toxic materials had been published by HELLING *et al.* (25). Further analytical studies using gas chromatography with detection and identification by mass fragmentography had been reported by BUSER and BOSSHARDT (26). The method, with a limit of determination in the $\mu\text{g/kg}$ range, was used to monitor samples of 2,4,5-T from European manufacturers.

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Appendix II: Residue Analysis of Organophosphorus Compounds

The last comprehensive review of progress in residue analytical procedures for compounds which were under evaluation by the FAO-WHO JMPR was presented to the 1970 meeting (FREHSE 1971a). In the meantime, additional compounds had been evaluated by the JMPR. Table 1 gave a complete list of organophosphorus insecticides, acaricides, and nematocides, which were of current interest to the JMPR and/or the FAO-WHO Codex Alimentarius Commission on Pesticide Residues, up to and including the 1974 JMPR. Capital letters attached to the individual compounds were explained in the text (see *Multiresidue Methods*).

Table 1

Azinphos-ethyl			D ¹	E	
Azinphos-methyl			D ¹	E	
Bromophos-ethyl			D		
Bromophos-methyl			D	E	
Carbophenothion	A ²	B	D	E	
Chlorfenvinphos			D	E	
Chlorpyrifos					S
Coumaphos					S
Crufomate					S
Demeton			(D)*		S

Demeton-methyl and Oxydemeton-methyl				(D)*		S
Diazinon	A	B	C	D ¹	E	
Dichlorvos				D		
Dimethoate				D	E	
Dioxathion				D	E	
Disulfoton				D*	(E)*	
Ethion	A	B		D*	E	
Fenamiphos						S
Fenchlorphos	A			D	E	
Fenitrothion				D	E	
Fensulfothion						S
Fenthion				D*	(E)*	
Formothion				D	E	
Malathion	A	B	C	D ¹	E ¹	
Methodathion						S
Mevinphos				D	E	
Monocrotophos						S
Omethoate				D		
Oxydemeton-methyl	See demethon-methyl					
Parathion	A	B	C	D ¹	E	
Parathion-methyl	A	B	C	D ¹	E	
Phosalone				D		
Phosphamidon				D		
Pirimiphos-methyl						S
Thiometon				D*		
Trichlorfon				D		
Trichloronat						S
Vamidothion						S

Additional compounds covered by some of these methods:

Dichlofenthion	D	
Dimefox	D	
Ethoate-methyl	D	
Mecarbam	D*	
Naled (dibrom)	D	
Phenkapton	D	E
Phorate	D*	
Pyrimithate	D	
Sulfotep	D	
Zinophos (thionazin)	D ¹	E

¹ oxon included

² low recoveries might be encountered

* significant oxidative metabolites included

() * significant oxidative metabolites *not* included

This report was confined to recent advances in residue analytical methodology concerning the compounds listed in Table 1. It aimed at representing a critical selection of available methods and was, therefore, not intended to be a review-type paper covering the entire literature relating to these organophosphate pesticides. For the same reason, publications not resembling complete methods of analysis or methods based on tlc or other techniques not in wider usage for routine analysis, had also been neglected. This principle was followed in order to underline the advisory character of the Commission's activity. In future, authors of pertinent analytical procedures would be asked whether their method would meet with the validation requirements as outlined in this paper. For next year's meeting, the list presented here would then be expanded accordingly.

Multiresidue Methods. There was an increasing number of publications dealing with the simultaneous determination of a multitude of residues. In the

absence of indications to the contrary, it must be presumed that a great number of these procedures had not yet been validated in laboratories outside the author's premises. Such methods could not be recommended for general use for the time being because the recommendation of analytical methods should not, wherever possible, be based on unilateral experience. Institutions or individuals who had practical experiences of such methods, were invited urgently to inform the Commission Chairman accordingly so that additional multiresidue procedures could be added to the recommendation. Another prerequisite for recommending a multiresidue procedure was that adequate recoveries could be demonstrated and that significant metabolites, *i.e.*, those known to contribute to the biological efficacy of a product (*e.g.*, sulfoxides and sulfones deriving from thioether compounds, some oxons deriving from dithio- or thiono-parent compounds) or to be of toxicological significance, were included in the analytical procedure.

The following procedures had been taken into account. The capital letters in Table 1 indicated the compounds to which the method was demonstrated to be applicable.

- A. General method for chlorinated and phosphated pesticides, AOAC (11th Ed.) 29.001-29.027.
- B. Multiple residue method for phosphated pesticides, AOAC (11th Ed.) 29.028-29.033.
- C. Single sweep oscillographic polarographic confirmatory method (for A), AOAC (11th Ed.) 29.034-29.038.

Table 2. Crops which can be analyzed by methods as stated (A, B, and E)

	A	B	E
Apples	A		
Apricots	A		
Barley	A		
Beans			E
Beets	A		
Broccoli	A		
Cabbage	A		E
Cantaloupe	A		
Carrots	A	B	E
Cauliflower	A		
Celery	A		E
Cherries			E
Corn (silage)	A		
Cucumbers	A		
Eggplant	A		
Endive	A	B	
Grapes	A		E
Kale	A	B	
Lettuce	A	B	E
Oats	A		
Peaches	A		E
Pears	A		E
Peppers (green)	A		
Plums	A		E
Potatoes	A	B	
Radishes	A		
Spinach	A		
Squash	A		
Strawberries	A	B	E
Sweet potatoes	A		
Tomatoes	A		
Turnips (incl. greens)	A		
Wheat	A		
Various 'greens' of minor importance	A		E

Method D was designed for total diet studies and was, therefore, applicable to a great variety of food commodities.

- D. ABBOTT *et al.* (1970). This method was still valid in basically unaltered form (ABBOTT, 1974). For more recent published versions of the method as applied to cereals, see CRISP and TARRANT (1971) and the Panel Report (1973). Concerning the extraction and cleanup steps, the following modifications were in use (ABBOTT 1974):

Group 1 crops (cereals). 10 g of sample now taken instead of 50 g, mixed with 5 g of anhydrous Na_2SO_4 (except for cereal grain) and macerated with 3 aliquots of methanol (50 ml each). The 3 fractions were collected in a centrifuge bottle and centrifuged for 4 minutes, poured through a cottonwool plug, and evaporated to 2 ml, using an air blast or a micro-snyder column. The volume was then made up to 10 ml with acetone.

Group 2 commodities (meats and fish). 10 g of sample now taken instead of 50 g; extraction procedure unaltered.

Group 3 commodities (fats and butter). 5 g of sample now taken instead of 50 g and extracted 4 times with petroleum ether 60-80° C (50 ml each); the extracts were collected in a 500-ml separatory funnel and separated with 3 aliquots of acetonitrile (50 ml each). Further procedure was then as for Group 2.

Groups 4, 5, and 6. 20 g of sample now taken instead of 50 g; extraction procedure unaltered.

Group 7 (milk). 30 g of milk now taken instead of 50 ml. Extraction as for Group 2.

Note. In all methods involving the use of acetonitrile, the Kuderna-Danish evaporator must be modified by substituting the fractionating column by a Quickfit stillhead with a condenser connected to it. If a 'true' K-D was used, the acetonitrile was preferentially concentrated and could not be eliminated.

Another modification of the UK Laboratory of the Government Chemist Method (ABBOTT *et al.* 1970) for application to fruits and vegetables was currently being studied (ABBOTT 1974). The major alteration was the use of a 5-ft column of 3% OV-17 on 60-80 mesh Gas-Chrom Q (pre-conditioned at 265° C in the usual manner and, additionally, with dimethoate and azinphos-methyl if these compounds were to be determined). Column temperatures were 180° C for DDVP; 220° C for dimethoate, malathion, and parathion; 240° C for azinphos-methyl. Further experiences with this modification should be awaited before it was recommended for general use.

- E. G. BECKER, Method S 8, in *Deutsche Forschungsgemeinschaft, Rückstandsanalytik von Pflanzenschutzmitteln*, 3. Lieferung 1974, Verlag Chemie, Weinheim/Bergstr.

- S. See under *Special Methods*

Table 2 indicated that most of the compounds could be determined, in a great variety of commodities, with the five methods which had been selected for the purpose of this review.

Special Methods. The significance of Special Methods and their relation to multiresidue procedures had been discussed or outlined repeatedly in recent years (FREHSE 1970, FREHSE 1971b, FAO-WHO 1972, IUPAC 1972). There

was a general and justified tendency to prefer multiresidue procedures for all practical purposes of food inspection or tolerance enforcements. For 'academic' studies on the behaviour of a given pesticide in the environment*, or—in particular instances—in 'cases of dispute', it might be preferable to use a special method. However, these methods hardly lent themselves to generalized recommendations, because in the light of their very particular importance they were often subject to frequent revisions or modifications in order to keep them adjusted to current or extended demands. For the specific purposes of their application, it might, therefore, be more advisable for institutions or interested individuals to contact laboratories known to have the best possible knowledge about the latest developments in methodology (e.g., the residue laboratories of a main manufacturer) rather than to rely exclusively on such methods in the form in which they were published.

For these reasons, the 'validation aspect' as expressed earlier could not always be maintained when selecting or proposing special methods. The other requirements which were outlined as governing the selection of multiresidue procedures did, of course, also apply here.

The Commission might, therefore, wish to adopt a policy of recommending or proposing special methods for general use, solely for two reasons:

1. a suitable and validated multiresidue method was not available for the compound in question;
2. the occurrence of significant metabolites which, for various possible reasons, were not normally included in a multiresidue method, made it necessary to use a special method for clarification. Such necessities should, however, be brought to the attention of the Residue Analysis Commission, either from the Terminal Residues Commission or from any other competent source, so that the Residue Analysis Commission could then take suitable measures.

Chlorpyrifos was extensively evaluated by the 1972 JMPR. Numerous methods for various substrates were listed in the Monograph, including a flow diagram of three extraction and cleanup procedures generally suitable for (i) water, (ii) wet tissues and soil, and (iii) dry and fatty tissues, followed by glc (afid). The JMPR concluded that these procedures 'would be suitable for most regulatory purposes'. Unfortunately, they were described only qualitatively in the Monograph.

Recent methods not covered by the JMPR monograph were:

- (a) Sweep codistillation followed by glc with alkali flame ionization detector (afid) (MAINI and COLLINA 1972; MAINI *et al.* 1972). This procedure was suitable for plant material [apples, carrots, cauliflower, maize, kernels, lettuce, onions, oranges (pulp and peel), potatoes, soil, sugar beets (roots and leaves), tobacco]. It was essentially identical with the AOAC method (B, Table 1). The oxon was not detectable by this procedure, but it very rarely occurred in plants and animals.
- (b) Determination of parent compound and its oxon in cattle and turkey tissues and organs by glc with flame photometric P-detector (Ivey *et al.* 1972, MANN *et al.* 1973). A Russian glc method [electron capture detector (ecd) or afid] for determination of the parent compound—together with diazinon—in milk and organs and tissues of animals was also available (TALANOV and LESHCHEV 1972).

*The method of STELLER and BRAND (1974) on the analysis of dimethoate-treated grapes for *N*-hydroxymethyl and des-*N*-methyl metabolites and for their sugar adducts was perhaps a good example for this type of method development; see also under *Mono-crotophos*.

(c) Determination of parent compound and its oxon in wheat plants, kernels and straw by glc with flame photometric P-detector (STRUBLE and McDONALD 1973). With certain liquid phases, poor resolution of the two compounds (parent and oxon) or poor response of the oxon was encountered. STRUBLE (1973) studied these effects, comparing 10 polyalkyl glycol liquid phases. The most suitable material was Ucon 75-H-90,000.

BRAUN (1974), in trying to avoid this problem, developed a different procedure. After partitioning, the parent compound was eluted from a silica gel column prior to eluting the oxon in the form of its hydrolysis product (3, 5, 6-trichloro-2-pyridinol). Both compounds were then determined by glc, the parent with a flame-photometric detector (P- or S-mode), the pyridinol, after silylation, with an ecd. The method allowed also for the determination of free pyridinol, if present, in the same manner. Good recoveries were reported for the three compounds from vegetables (lettuce and celery). (This method was also suitable for the simultaneous determination of leptophos and its corresponding metabolites.)

All of these recently published methods appeared to be recommendable.

Coumaphos was evaluated by the JMPR in 1968. At that time, the glc method published by BOWMAN *et al.* (1968) appeared to be the method of choice. However, the meeting considered it desirable that collaborative studies should be made 'to evaluate its suitability as a referee method'. Apparently this was not done (*cf.* reevaluation by the 1972 JMPR). However, another glc method with flame photometric detection was developed for determination of coumaphos and its oxon in eggs (THORNTON 1968). It could also be applied to animal tissues and milk (OLSON 1971). The liquid phases used in these three methods were 10% DC-200, 5% DC-200, and 5% QF-1, respectively, on Gas Chrom Q.

Cruformate was evaluated by the JMPR in 1968 and 1972. Reference was made to an unpublished glc method for residues in animal tissues (RICE and DISHBURGER 1970) and the following statement was made (1972): 'The method has many features in common with existing multiresidue methods so it would appear reasonable that cruformate would be detected by these methods; this assumption, however, must be verified by collaborative testing.'

A method for the determination of residues in milk (glc with flame photometric detection) which was described by BOWMAN and BEROZA (1967b), would be suitable for regulatory use. Another glc procedure, employing an afid, for the determination of residues in bovine blood was published by GREENHALGH *et al.* (1972).

Demeton and Demeton-S-methyl and their Oxidative Metabolites (including Oxydemeton-methyl). Methods which could be recommended for wider regulatory usage were not yet available. The referee might be able to make suitable suggestions for the 1975 meeting. For a discussion of the methods currently in use, see 'Demeton-S-methyl—and related compounds' and 'Disulfoton' Monographs of the 1973 JMPR (FAO-WHO 1974).

Fenamiphos. THORNTON (1971) developed a method by which the compound and its sulfoxide were oxidized to the sulfone, and final determination of the sulfone was accomplished by glc with an afid. Typical substrates for which good recoveries were reported included milk, liver, citrus, peanuts, pineapples, tobacco, soil. With only minor modifications, this method was also applicable to broccoli, brussels sprouts, cabbage, cauliflower, carrots, cottonseed, lettuce, potatoes, soybeans, sugar beets, sweet potatoes and tomatoes. BOWMAN (1972) published a procedure, including light chroma-

tography, by which the three compounds could be determined separately in grass (glc with flame photometric detector). For practical purposes, the determination of the combined residues as a single peak seemed preferable.

Fensulfothion. Available glc methods were discussed and evaluated by the 1972 JMPR, which concluded that they 'are suitable for regulatory purposes as required'. This statement did not refer to methods which were developed for the determination of individual metabolites. The other methods were based on the principle of oxidizing fensulfothion, its sulfone, and its oxygen analogue to the oxon-sulfone, so that the combined residues were specifically measured as a single peak with an afid:

(a) maize (kernels, cobs, greens), peanuts, soil: KATAGUE and OLSON (1969), OLSON (1970), OLSON (1968), respectively

(b) bovine tissues and organs: THORNTON and OLSON (1968)

(c) tobacco: OLSON (1969)

Two of these methods were also used for analyzing bananas, pineapple, onions, potatoes, rutabagas, soybeans, sugarcane, sweet potatoes (KATAGUE and OLSON; with only minor modifications) and sorghum, grain, and forage, dry and fresh (OLSON 1970).

Methidathion. The method of EBERLE and HÖRMANN (1971), according to the JMPR 1972, appeared satisfactory for regulatory purposes. It was applied successfully to apples, cherries, grapes, hops, prunes, potatoes, and soil. Other methods were not available.

Monocrotophos. According to the 1972 evaluation of the JMPR, the glc method of BOWMAN and BEROZA (1967a) was still the method of choice for regulatory purpose. It was developed for whole sweet corn plants and worked with a flame photometric P-detector. Modifications of this method for application to other crops were demonstrated in various, although unpublished reports of Shell Research Ltd.; similarly, Shell had available reports on the employment of the afid for residue analysis in crops. BEYNON *et al.* (1973) published a method for determining neutral conjugates of an *N*-hydroxy-methyl derivative of monocrotophos.

Pirimiphos-methyl. No method available in the open literature.

Trichloronat. Because the oxon would occur, if at all, only in low concentrations, determination of the parent compound alone was sufficient for regulatory purposes. The methods developed by MÖLLHOFF for determining residues of pesticides belonging to the parathion group, using electron capture (1967) or thermionic (1968) detection, were recommended.

Vamidothion. A glc procedure had been developed by the manufacturer's laboratories. After suitable cleanup, the parent compound and its sulfoxide were oxidized to the sulfone which was determined with an electron capture detector (DESMORAS *et al.* 1972). Identity could be confirmed, and the parent compound and the sulfoxide separately determined semiquantitatively, by tlc (Rhône-Poulenc 1972). The glc method was considered suitable for regulatory purpose by the 1973 JMPR (FAO-WHO 1974); see respective monograph for a brief outline of the procedures mentioned, however, the substrates which could be analyzed by these methods were not given.

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Appendix IV: Residue Analysis of Insecticidal Carbonates

The determination of residues of carbofuran and its metabolites had received attention from various workers. WILLIAMS and BROWN (1) had published a glc method for residues on soft fruits. Although several methods had been published and various crops had been analyzed, there had been no previous study of carbofuran in small fruits. This method used a modified form of the extraction method of COOK *et al.* (2). Following dichloromethane extraction, silica gel and alumina column chromatography, samples were determined by glc with a Coulson conductivity detector in the nitrogen mode. Recoveries of both carbofuran and 3-hydroxycarbofuran from fortified samples were greater than 86% over the 0.2-5.0 mg/kg range. For carbofuran residues in soil, CARO *et al.* (3) used acid ammonium acetate extraction and glc with an electron capture detector. Determination at the 0.1 mg/kg level without cleanup was possible by formation of the dinitrophenylether derivative. Recoveries from various soils were in the 61-92% range. This method might prove useful because landrin, propoxur, and bux insecticides might also be determined. MOYE (4) studied the reaction between the phenolic portions of hydrolyzed carbamate pesticides and various aromatic sulfonyl chlorides. The resulting esters were highly sensitive to the electron capture detector. A method for carbofuran in lettuce at the 0.01 mg/kg level resulted from this work. Tlc and autoradiography techniques (5, 6) had been used to detect the breakdown products of carbofuran, such as carbofuranphenol, 3-ketocarbofuran, and 3-hydroxycarbofuran.

The direct glc of insecticidal carbamates was normally difficult because of thermal decomposition. A direct glc method, without cleanup, for carbaryl and its hydrolysis product 1-naphthol, had been published (7). This method was useful for quantities in the 0.2-15 ng range. A column (0.3 m x 4 mm) of 3% S.E.30 on 80/100 gas chrom Q was employed and no decomposition below 160° C was detected. The short column with a low loading was used to avoid errors resulting from decomposition. When examining water extracts for residues, no cleanup was found to be necessary. Carbaryl was generally determined by decomposition to 1-naphthol, forming a suitable derivative, and estimation by gas chromatography with an electron capture detector. The

pentafluorobenzyl esters and ethers had been used for the analysis of trace organic acids and phenols in water supplies, but the need for removal of excess pentafluorobenzyl bromide reagent was a drawback. JOHNSON (8) used the same derivatives, but removed excess reagents by the use of a silica gel column. He determined 1-naphthol and sec-amyl phenols, which were hydrolysis products of the insecticides carbaryl and Bux, respectively. The colorimetric method of AOAC (1970), depending on the formation of the *p*-nitrobenzene diazonium fluoroborate derivative, was used by KURTZ and STUDHOLME (9) to detect residues of carbaryl in birds; the minimum amount that could be detected was 0.1 mg/kg.

The results of a useful study on the stability of carbaryl in aqueous media were reported by WAUCHOPE and HAQUE (10). Carbaryl was found to be stable in weakly acidic solutions, but hydrolyzed to 1-naphthol under basic conditions. A similar study was conducted by MACNEIL *et al.* (11) for the compounds carbaryl and Mobam. The analyses for the decomposition products were carried out *in situ* on silica gel thin-layers by reflectance spectroscopy after the developed chromatograms had been sprayed with CNTNF(9-dicyano-methylene 2,4,7-trinitrofluorene) to form visible π complexes. CLEGG (12) reported a glc method for residues of promacyl in the tissues of cattle. The phenol produced by hydrolysis of the carbamate was coupled with fluoro-2,4-dinitrobenzene and determined by electron capture glc; the procedure was similar to that of COHEN *et al.* (13). However, important differences in the cleanup and reaction conditions during derivitization were developed in order to separate promacyl from its metabolites promecarb and isothymol. Recoveries for spiked samples were in the 80-90% range with a detection limit of 0.1 mg/kg. This method should be applicable to other aryl esters of carbamic acid.

A specific glc method for the determination of residues of mesurol and its sulphoxide and sulphone metabolites in plant and animal tissues was reported by THORNTON and DRAEGER (14). After initial extraction and precipitation cleanup stages, the extract was oxidized with potassium permanganate to convert mesurol and its sulfoxide to the sulfone. Final detection of the sulfone was by a sulfur specific flame photometric detector, thereby avoiding interference from tissue coextractives. The detection limit was 0.03 mg/kg.

To aid the analysis of pesticidal carbamates an understanding of the metabolism and degradation was both desirable and useful. MEIKLE (15) had reviewed the metabolism of Mexacarbate in biological systems and BENEZET and MATSUMURA (16) determined the major metabolites of this compound using ring labelled mexacarbate with silica gel tlc. UNGER and coworkers (17-19) studied the photochemical breakdown of mexacarbate, metacrate, maticil, and landrin. A detailed analysis of the metabolites and residues resulting from the soil application of aldicarb under field conditions had been reported by ANDRAWES *et al.* (20). The procedure was based on determination of the aldicarb sulfoxide and sulfone metabolites as the sulfones after oxidation by perchloric acid. Two-dimensional tlc was used to resolve the various metabolic components present in organic extracts of plant samples. The methods described were useful for characterizing aldicarb residues in cotton foliage and for determining the total toxic residue at a level of 0.01 mg/kg in cotton seed. The flame photometric detector was also used by WOODHAM *et al.* (21) for examining the effect of aldicarb sprays on grasses and wildlife. WHITTEN and BULL (22) investigated the fate of a recently introduced carbamate insecticide Diamond Shamrock DS 15647 [3,3-dimethyl-1-(methylthio)-2-butanone *O*-(methylcarbamoyl)oxime] in cotton plants and

soil using the labelled insecticide, the breakdown metabolites being separated and identified by tlc and radiography.

A detection limit of 0.05 mg/kg was achieved by REEVES and WOODHAM (23) when determining residues of methomyl in soil, sediment, and tobacco, by glc with a flame photometric detector after Florisil cleanup. MENDOZA and SHIELDS (24) reported a method for methomyl in rapeseed oils by glc with electron capture detection of the DNFB-methylamine reaction product after cleanup on a silica gel microcolumn. To ensure complete hydrolysis of the carbamate, sodium hydroxide was added immediately before reaction with DNFB. Recoveries at the 0.01-1 mg/kg level were 80-105% and no glc interference was obtained from the oil. The optimum conditions affecting the DNFB and methylamine reaction were also studied. Details of the micro-column cleanup technique for the rapid cleanup of the reaction product extracts were subsequently published (25). MENDOZA *et al.* (26) developed a tlc enzyme inhibition technique for the semiquantitative detection of methomyl residues in rapeseeds, oils, and meals. The method was suitable for the detection of methomyl, but not the oxime, at a detection level of 20 ng in the presence of extractives. Tlc with iodo- or chloroplatinate reagents was also used for confirmation; although 50 times less sensitive than the enzyme reaction for methomyl, it also detected the oxime.

Data on the metabolism and residues of methomyl in the rat, tobacco, corn, cabbage, and soil, provided at the time of registration of this compound in USA had been published in three papers by HARVEY *et al.* (27-29). The authors used temperature programmed glc and tlc with mass spectrometry-infrared for identification.

CHENG and CASIDA (30) used tlc with a variety of solvent systems and visualizing agents to identify the metabolites and photoproducts of radio labelled BPBSMC[3-(2-butyl)-phenyl *N*-benzenesulfonyl-*N*-methyl carbamate] and BPMC[3-(2-butyl)-phenyl *N*-methyl carbamate]. Product confirmation involved a variety of procedures including infrared, mass spectrometry, and nuclear magnetic resonance spectrometry. Liquid scintillation spectrometry was also used for the determination of radioactivity. The value of this paper was enhanced by the inclusion of procedures for the radiosynthesis of the parent compounds together with their degradation products.

Multiresidue Methods. Since the 1973 report there had been considerable activity in the development and application of analytical techniques and systems for the multiresidue determination of carbamates.

FREI *et al.* (31) developed a scheme for carbamate insecticides by combining fluorogenic labelling and high performance liquid chromatography. The formation of the dansyl chloride derivatives allowed a wide range of *N*-methyl carbamate insecticides to be separated at detection limits between 1-10 ng per 4- μ l injection (fluorescence detector); soil and water samples containing mesurol and carbofuran could be determined without the need for a preliminary cleanup stage. Development of a multiresidue method based on the technique of FREI *et al.* (31) would be desirable because this would be useful for total diet samples. A procedure for pesticide residues including phenyl and methyl carbamates in plant material had been published by THIER (32). Following separation from other pesticides by Florisil column chromatography, the carbamates were determined by electron capture glc after bromination. SUZUKI *et al.* (33) developed a systematic procedure for the separation and identification of a mixture of 13 carbamate pesticides. After separation on silica gel tlc plates, trifluoroacetates were prepared and identified by glc. ISHIKAWA (34) established an analytical method for the separation and

determination of insecticidal carbamate residues in rice grain. Following hexane-acetonitrile partitioning and alumina column cleanup, the carbamates were hydrolyzed to their corresponding phenols and coupled with a 4-nitrobenzenediazonium ion to produce coloured compounds which could be separated and identified by tlc. Recoveries by 60-80% were obtained at the 0.1 mg/kg level for *N*-methyl carbamates except 1-naphthyl *N*-methylcarbamate. The formation of aromatic sulfonyl chloride esters (4) and fluoro-2,4-dinitrobenzene derivatives (2) previously mentioned were also suitable products for multiresidue separation and identification of certain insecticidal carbamates by glc.

Recommendations. The major problem with carbamate determination had been in the thermal instability of the compounds, thus making the application of direct glc difficult. The formation of halogenated derivatives had gone some way to overcoming this problem, but derivatization was often time-consuming and involved. The method of HOLDEN (35), as mentioned in the previous report, involving the glc of the 1-fluoro-2,4-dinitrobenzene derivatives of methyl carbamates, appeared promising and should be tested collaboratively. There was a great need for a method for multiple residues which was both rapid and specific. Finally, wherever chlorinated hydrocarbons were used for the extraction procedure, provision should be made to extract any water-soluble and conjugated metabolites which might be more potent cholinesterase inhibitors.

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Appendix III: Residue Analysis of Organophosphorus Compounds Reported in COMECON Countries

Residue Analysis of Individual Compounds. A number of papers on routine use of tlc for organophosphorus residues had been published since the last meeting. Methods were reported for residues of phosalone and phenthoate in apples (1, 2), and for phosalone, trichlorfon, parathion methyl, malathion, and dimethoate in soil (3, 4). A tlc method for phosalone and phosmet (6), and PC combined with colorimetry for fenchlorophos were used in forensic analysis (7). Residues of parathion, malathion, fenitrothion, dichlorvos, trichlorfon, fenthion, demeton methyl, dimethoate, and their toxic metabolites were determined in 16 fruit and vegetable species with a sensitivity of 0.01-1.0 mg/kg (8). A modified NBP reagent was reported (9) for the detection of omethoate, demephion, and metabolites. Tlc methods were described for residues of diazinon (10), Butiphos (DEF) in cotton, cotton seed oil (11), and groats (12), and for Trakephon (*O,O*-dibutyl-1-butalamino-cyclohexylphosphonate) in soil and potatoes (13).

A voltametric oscillopolarographic method with a sensitivity of 0.2 mg/kg was used for phosphorodithioate and carbamate residues in apples, following alkaline hydrolysis (14). A method of enzymatic titration was described (15) and used for the determination of Butiphos and Folex, respectively, in plants. The limit of detection was 2 μ g for Butiphos and 1 μ g for Folex. The sum of trichlorfon and dichlorvos residues in waste waters and natural water (16), and residues of dichlorvos in milk (17) were determined colorimetrically with a sensitivity of 0.05 and 0.1 mg/l. Rapid colorimetric methods were proposed for the determination of dimethoate and phosalone in air (18).

Multiresidue Methods. A procedure for the column extraction of organophosphorus (OP) residues based on the elution of a homogeneous mixture of the blended plant material with deactivated silica was used for 7 pesticides on 15 crops (19). The recoveries were evaluated by means of glc and a radioactive isotope technique, respectively, and ranged from 90 to 100%. OP residues in

citrus juice (20) and animal tissues (21) could also be extracted by this procedure.

In connexion with the glc-TID determination of OP residues, an adaptation of glc apparatus for the sweep codistillation cleanup of extracts was developed (22). The recovery was evaluated for a mixture of diazinon, malathion, fenitrothion, and trichloronat on 10 fruit and vegetable species, and in milk. The mean value (in %) for plants was as follows: diazinon (94.2), malathion (87.9), fenitrothion (84.1), and trichloronat (86.4); for milk the recovery was within the range 96-107%.

A glc-TID analysis following acylation for phosphonic acid esters was reported (23). An alkylation procedure at the microgram level was developed as a chemical confirmatory test for OP and carbamate insecticides, and *s*-triazine and urea herbicides with reactive NH moieties (24). TID, electron capture and flame ionization detectors were evaluated for OP and organochlorine pesticides (25). The minimum detectable concentrations of the pesticides were expressed in mg/sec for each detector type.

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Appendix V: Residue Analysis of Herbicidal Carbamates

Development of a satisfactory multiresidue methodology for the carbamate herbicides by direct chromatography was part of the overall difficult problem of developing such methodology for nitrogen-containing pesticides, mainly because of the tendency of these compounds to degrade on glc columns (1-3). Derivatization of either the carbamate compounds or their hydrolysis products, followed by glc determinations, had been suggested in the past and employed rather successfully (4-9).

Recently, direct chromatography of a number of the carbamate herbicides was reported by LASKI and WATTS (10). By employing carefully controlled chromatographic conditions, using the Coulson electrolytic conductivity detector, and a 5%- and a 10%-DC-200 column, these authors successfully minimized considerably the degradation and adsorption of carbamate herbicides, amongst other organonitrogen pesticides studied, on the glc columns. Table 1 summarized the glc data—relative retention times (RRT, parathion=1.00), and the amounts (ng) needed to cause a response of approximately 50% fullscale deflection (FSD) for the standard compounds chromatographed in these studies.

Table 1

<i>Compound</i>	<i>Chemical Name</i>	<i>RRT</i>	<i>ng for 50% FSD</i>
EPTC	S-Ethyl dipropylthiocarbamate	0.13	10
Propham	Isopropyl N-phenylcarbamate	0.16	10
Butylate	S-Ethyl diisobutylthiocarbamate	0.17	10
Vernolate	S-Propyl dipropylthiocarbamate	0.17	10
Pebulate	S-Propyl butylethylthiocarbamate	0.18	20
Cycloate	S-Ethyl cyclohexylethylthiocarbamate	0.31	20
Chlorpropham	Isopropyl N-(3-chlorophenyl) carbamate	0.31	25
Diallate	S-2, 3-Dichloroallyl diisopropylthio- carbamate	0.37; 0.39	50
Tandex	m-(3, 3-Dimethylureido) phenyl- <i>tert</i> - butylcarbamate	0.12; 0.42	75*
Sirmate (2, 3-isomer)	2, 3-Dichlorobenzyl N-methyl carbamate	0.54	40
Simate (3, 4-isomer)	3, 4-Dichlorobenzyl N-methyl carbamate	0.55	40
Triallate	S-2, 3, 3-Trichloroallyl diisopropyl- thiocarbamate	0.62	50

*Peak tailing occurs.

Procedures for cleanup of carbamate herbicide residues in crops for measurements by means of the Coulson detector were currently employed by

the US Food and Drug Administration. For residues of carbamate herbicides that were water insoluble and acetonitrile extractable, it seemed possible that the FDA multiresidue chlorinated pesticides procedures (11) might usefully be employed. The recent development of a highly deactivated column packing material—an acid-washed Chromosorb W support, surface-modified with Carbowax 20M (12)—had enabled the direct gas chromatographic analysis of some *N*-methyl carbamate pesticides using an alkali flame detector (13). In principle, the use of this column might also prove to be useful for the direct gas chromatographic analysis of *N*-methyl carbamate herbicides (e.g., Sirmate, Terbutol, Metham). A rapid screening method for determining Chlorpropham (CIPC, 3-chlorophenyl-isopropyl carbamate) at low residue levels in plant materials was described by FRIESTAD (14). This method utilized a preliminary cleanup with a slightly modified MILLS-ONLEY-GAITHER procedure (15), followed by hydrolysis of CIPC to the aromatic amine, which after automatic diazotization and coupling, was measured by colorimetry. LONG and THOMPSON (16), in a study of some herbicide residues in air-cured burley tobacco, could not detect under the extraction and detection techniques employed any residues of the carbamate herbicide Perbulate (*S*-propylbutyl-ethylthiocarbamate), which was applied at planting of tobacco and was persistent in the soil, possibly making it available for uptake by the tobacco plant. The limit of detection under the conditions used by these authors—a flame ionization detector and borosilicate glass columns packed with 10% OV-17 on 80-100 mesh Gas chrom Q—was 0.02 g/g of dry weight, including a 60% recovery value. Complete metabolism by the tobacco plant of the thiocarbamate herbicide was suggested as an explanation for the absence of residues of Perbulate.

The use of a radioassay technique for study of the uptake and metabolism by corn seedlings of the carbamate herbicide EPTC (ethyl-*N,N*-di-*n*-propylthiocarbamate) in an effort to elucidate also the mechanism of protection to corn from EPTC injury by the presence of *N,N*-diallyl-2,2-dichloroacetamide, was reported recently (17). In this study, plants treated with ¹⁴C-EPTC were extracted with 50% methanol, centrifuged, and aliquots of the supernatants were used directly for radioassay. Radioactivity in the pelleted residues was estimated by combustion in a Packard 305 sample oxidizer and subsequent liquid scintillation counting of the liberated ¹⁴CO₂. Radiolabelled metabolites in the aqueous phase were analysed by tlc on silica-gel G in BuOH-CH₃COOH-H₂O (4:1:1) and benzene-EtOH (75:25). Radioactive compounds on the tlc plates were detected by autoradiography and subsequent counting of the radioactivity in each spot. Radioassay techniques were also used in a study in the isolation and identification of Propham (isopropyl *N*-phenyl carbamate) metabolites from animal tissues and milk (18). In this study ¹⁴C-radiolabelled metabolites in goat milk, goat tissue, and chicken tissue, were isolated by solvent extraction and column chromatography, then identified by comparative spectrometry.

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Appendix VI: Residue Analysis of Fumigants

A limited number of publications of value in the advancement of analytical methods for fumigant residues had appeared during the past year.

Residues from Use of Phosphine. The aeration method of BRUCE, ROBBINS and TUFT (1) had been used to determine free phosphine in commodities by other workers (2) and appeared to be the method of choice. DUMAS and BOND (3) had shown, however, that when aluminium phosphide-generated phosphine was passed through a chromatographic column consisting of Apiezon L on firebrick, odourless phosphine was eluted, suggesting that there was also present an unidentified foul-odoured volatile compound capable of producing a residue for which no analytical method yet existed.

Residues from Use of Methyl Bromide

(a) *Bromide Ion.* Bromide had been determined in wheat and potato tubers (and haulm), using X-ray fluorescence spectrometry of pressed powdered samples by BROWN *et al.* (4) with a claimed sensitivity of 1 ppm (10 ppm in haulm). The glc method of HEUSER and SCUDAMORE (5) for specific determination of bromide ion in cereals was currently being tested collaboratively by 8 UK and Netherlands official laboratories. This method had also been adapted by GREVENSTUK (6) for the determination of bromide ion in milk.

(b) *Alkylation Reaction Products.* ASANTE-POKU *et al.* (7) had determined methylation sites in free amino acids and those from protein hydrolysates of cocoa bean shell and nib after fumigation with ¹⁴C-labelled methyl bromide, using a Beckman amino acid analyzer for separation and liquid scintillation counting of the separated fractions. Methylated basic amino acids were separated and provisionally identified by tlc.

Ethylene Oxide Residues. Two methods for determination of residual ethylene oxide in sterilized pharmaceutical materials, such as polymers, cotton, *etc.*, were compared by ROMANO, RENNER and LEITNER (8). Results obtained by extraction or solution with dimethyl formamide, with analysis of aliquots by gas chromatography with flame ionization detection were similar to those obtained by subjecting the sample to heating at 100°C in a sealed vial, followed by gas chromatography analysis of the headspace gas using Porapak R as stationary phase. A sensitivity of 0.1 ppm of ethylene oxide was claimed for the latter method. WHITE and BRADLEY (9) determined residual ethylene oxide

in similar materials by high-vacuum distillation followed by gas chromatography with flame ionization detection.

Residues of Halogenated Hydrocarbon Fumigants. Collaborative tests by 8 laboratories of the multiresidue detection method of HEUSER and SCUDAMORE (10), modified by use of gas chromatography column, consisting of 15% w/w polypropylene glycol on Chromosorb W, had been completed. Two series of tests, the first using wheat and maize fumigated with carbon tetrachloride and the second in which a mixture of chloroform, trichloroethylene, and ethylene dibromide residues was similarly recovered, had been described for publication in *The Analyst* in 1974.

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Appendix VII: Residue Analysis of Systemic Fungicides

Since the last report in 1973 only a few new residue methods had become available for the systemic fungicides. The first gas chromatographic method for the determination of benomyl was published by ROUCHAUD and DECALLOME (6). Residual benomyl and MBC were extracted with benzene and partitioned into 0.1N hydrochloric acid. The acidic layer was washed several times with chloroform, then neutralized. All benomyl was converted to MBC by the extraction and cleanup and partitioned into ethyl acetate. MBC was then trifluoracetylated and measured by glc using an electron capture detector. The lower limit of detection was reported to be 0.02 ppm. Recoveries of 80-100% were achieved.

The determination of benomyl in the presence of thiabendazole, using a spectrofluorimetric method after column chromatographic cleanup with a magnesium oxide-celite-alumina column, had been published by AHARONSON and BEN AZIZ (1). Detection limits of 0.1 ppm for benomyl and 0.02 ppm for thiabendazole were reported. A tlc determination after a cleanup by a partition process with ethyl acetate was published by TJAN and BURGERS (7). Thiabendazole could be determined along with benomyl. For the simultaneous detection of benzimidazole fungicides in the presence of carboxin, oxycarboxin, tridemorph, dimethirimol, and ethirimol, BAKER and HOODLESS (2) also recommended tlc on silica plates or alumina plates. Thiabendazole could be determined generally following the UV-spectrophotometric procedure described for benomyl and MBC. A recent paper by RAJZMAN and BET DAGAN (5) described this procedure.

Recommendation (benomyl and MBC). From our own experiences and other sources (DRESCHER, VIEL) it seemed that for residue analysis the extraction of the substrate was performed advantageously with ethyl acetate. The residue was reextracted with hydrochloric acid and partitioned from the solution (pH 4.5) into ethyl acetate, reextracted with hydrochloric acid, and determined by UV-spectroscopy. This procedure led to satisfactory results for most crops. An additional test by one of the mentioned tlc assays gave necessary confirmation and indicated the presence of interfering substances. The new gas chromatographic determination gave a promising alternative with a more specific determination. However, using benzene as an extraction solvent was somewhat contradictory to the common procedure of using ethyl acetate. It was recommended to give this method more attention in the forthcoming work.

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Appendix VIII: Residue Analysis of Dithiocarbamate Fungicides

Few works on residue methodology for ethylene thiourea (ETU), a decomposition product common to some major dithiocarbamate fungicides, and on specific determination of one dithiocarbamate fungicide, had become known since the last IUPAC review on this subject.

The specific residue analysis of thiram (tetramethyl-thiuram disulfide) was reported in a few studies. KETTMAN and his coworkers (1), applied infra-red multiple attenuated total reflectance (matr) spectrometry to the identification and measurement of thiram residues on lettuce. By comparing spectra of extracts obtained from lettuce leaves free from thiram or enriched with thiram (80 μg per 100 g of leaves), and of the spectrum of thiram (20 μg) deposited directly on a KRS-5 crystal, it was shown that the fungicide could be identified satisfactorily at a concentration of 1 ppm in the sample.

RAPPE, MAUQUOY and BAUR described recently (2) a microbiological method for the determination of thiram residues. These authors claimed to have developed a rapid and simple agar plate method for the determination of thiram, using *Saccharomyces carlsbergensis* ATCC-9080 as the test organism. With this organism, as little as 25 ng of thiram/well or 200 ng/disk could be detected. The authors pointed out that this method was highly sensitive and could be applied when the nature of the fungicide being investigated was known. Other dithiocarbamate fungicides with antibacterial properties, such as nabam and ziram, could also be determined by this method but at higher concentrations than with thiram, and thus would not interfere with the thiram assay. In the chemical methods for the determination of thiram, such as the colorimetric method reported by RANGASWAMY (3), the presence of ziram and ferbam in the sample analyzed would cause an interference.

LASKI and WATTS (4) in their investigation on the determination of 95 organonitrogen pesticides in a glc system with the Coulson electrolytic conductivity detector, could not get any response to a 200-ng injection of ziram, used as a model in this study for the behaviour of other metallic dithiocarbamate fungicides.

A polarographic technique for measuring ETU residues in crops and animal substrates with a reported sensitivity of about 0.05 ppm, was developed recently by ENGST and SCHNAAK (5). In this technique, ETU, after cleanup separation with the aid of column and paper chromatography, underwent nitrosation and was measured by the use of a cathode ray polarograph. A tlc detection technique for ETU was described during the Helsinki Pesticide Chemistry Congress (6), whereby ETU, after nitrosation, was reacted with the Bratton-Marshall reagent [*N*-(1-naphthyl)-ethylenediamine dihydrochloride] for visible tlc spotting.

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Appendix IX: Residue Analysis of Rethrin and Synergist

It had been stated that the requirements of the FAO-WHO JMPR for methods of residue analysis of rethrins and synergists had been met (1), but this appeared not to be so. In addition, the greatly renewed interest in pyrethrum and synthetic pyrethroids as environmentally acceptable replacements for more persistent and more toxic pesticides might result in the need for and development of new methods of analysis which the Residue Analysis Commission would review.

The photodecomposition of resmethrin and related pyrethroids was studied by UEDA *et al.* (2), who found that the mammalian toxicity of photodecomposed resmethrin depended on the route of administration. The toxicity to mice of mixed photoproducts via intraperitoneal administration was greater than resmethrin, but less when administered orally. From these results one concluded that residue analysis for the parent compound only continued to be valid. A tlc procedure for the identification and quantitation of pyrethrins and piperonyl butoxide was developed by OLIVE (3). Treatment of the tlc plate with a mixture of phosphoric, tannic, and acetic acids, in acetone resulted in pink spots for pyrethrins and a blue spot for piperonyl butoxide. Although the method was developed primarily for formulation analysis, it could determine 1 µg of either compound and should therefore be suitable for residues with adequate cleanup.

A spectrophotometric method for the microdetermination of piperonyl butoxide in the presence of pyrethrins was developed by BHAVNAGORY and AHMED (4). Treatment of the mixed residue extract with 18% nitric acid

converted the piperonyl butoxide into a soluble yellow compound with an absorption maximum at 370 nm. The method was sensitive to 4 μg of piperonyl butoxide per ml of measurement solution. A novel procedure for determining resmethrin in peanuts was given in an application note for plasma chromatography (5). A cleaned up extract of 25 g of peanuts containing 0.1 mg/kg of resmethrin in 100 ml of solvent was analyzed by gas chromatography (OV-17 column at 200°C) interfaced with a plasma chromatograph (PC) as a selective detector. When 5 μl of extract containing 1.25×10^{-10} g of resmethrin was injected with the plasma chromatograph tuned to the characteristic drift time of resmethrin, a peak was observed at a gas chromatographic retention time of 6 minutes. A signal to noise ratio of 25/1 was obtained on the PC, whereas the flame ionization detector on the gas chromatograph gave no response at the low levels. No information was given as to whether the response (area) was proportional to concentration.

A microanalytical procedure for determining residues of Bioethanomethrin^R, [(5-benzyl-3-furyl)methyl IR, 2R-2 (cyclopentylidene)methyl]-3,3-dimethyl-cyclopropane carboxylate, a new synthetic analogue of pyrethrin, was developed by GEORGE and McDONOUGH (6). The molecule was saponified in alcoholic sodium hydroxide and a trichloroacetyl derivative made from both the resultant acid and alcohol. The carboxyl group of the acid was protected during esterification with trichloroethanol by pretreatment with dicyclohexylcarbodiimide in pyridine. The derivitized esters were then determined by gas chromatography using an SE-30 column. Usable response from an electron capture detector was obtained from as little as 0.6 ng of either ester. Application of the method to crop extracts was under investigation.

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Appendix X: Selective Gas Chromatographic Detectors

Introduction. Sensitivity, selectivity, linearity, speed, and ruggedness were the criteria generally used to judge detector performance. Significant improvements in these categories had been achieved on a variety of detectors in recent years. Yet, these did not always filter through the instrument manufacturers to the users as fast as would be desirable—nor was it uncommon to find some detectors, notably ec and afid, operating at less than optimum conditions in analytical laboratories.

Electron Capture Detector (ecd). This detector could be operated in DC, pulsed, or a new mode called 'linearized', 'frequency-modulated', or 'constant current' electron capture (1). Calibration curves for the latter were linear over four decades with argon-methane as a carrier gas. In order to use nitrogen, or to work at the highest possible sensitivity, some of this linearity had to be sacrificed. Several gas chromatography firms now sold the electronics

necessary for this new ec mode, and the detector was used increasingly in residue laboratories. Although it was too early yet for a final judgement on its performance in routine analysis, prospects looked good. The detrimental effect of oxygen—contained in the carrier gas or diffusing in from the atmosphere—should again be stressed (2). A suitable oxygen scavenger and a 'clean' chromatographic system were of paramount importance for good ec performance. The condition of any ecd could easily be judged by I/V plots in the DC mode or I/frequency plots in the pulsed mode. It was deplorable in this context that some ec detectors on the market did not provide for easy variation and readout of the potential used in DC mode. A recent review by this author was cited as reference (3).

Alkali Flame Ionization Detector (afid). Afid was most useful for phosphorus- and nitrogen-containing compounds, in competition with the flame photometric and the electrolytic conductivity detector, respectively. Afid was generally the cheapest, most sensitive, least selective, and least rugged of the three. Thus, further industrial development centred on the latter two parameters, and included the long known use of a mobile collector electrode (4, 5), the noise-reducing function of an auxiliary polarizing electrode (4), and the development of more stable alkali sources, for instance a rubidium glass bead (6). Afid was the one detector most in need of frequent optimization and constant surveillance. Two older reviews of its constructions and functions could be found in references (7) and (8).

Flame Photometric Detector (fpd). Since the pioneering work of BRODY and CHANEY and of BOWMAN and BEROZA, very little detector development *per se* had taken place. Noteworthy, however, was the recently described approach to switch (and carefully adjust) the gas flows such that hydrogen was mixed with the carrier gas before combustion. The signal/noise ratios were not significantly changed, but the bothersome extinguishing of the flame—which called for bypassing the solvent peak or relighting the flame—was now eliminated (9). Although used with *liquid* effluents, the successful wedding of the fpd to a wire transport system for determination of phosphorus pesticides needed at least to be mentioned here (10).

Electrolytic Conductivity Detector. In this area improvements were the most pronounced. Peak broadening had been curtailed and sensitivity had been markedly improved (11, 12). The company, which marketed the Coulson detector, now promoted the 'Hall Detector'. It was apparently quite convenient to use and at least ten times more sensitive than the older models (13). From what was known now, the improved conductivity detector might well find increased use in the analysis of nitrogen- and sulfur-containing compounds at the expense of afid and fdp, respectively. Its sensitivity was similar to that of the other detectors, and selectivity against carbon was much higher. One technique, however, for which this author would prefer the quicker responding flame detectors, was high-resolution gas chromatography. In regard to polychlorinated hydrocarbons, the Hall detector would compete well with ecd in cases where the superior sensitivity of the latter was not required, but where polar coextractants called for improved selectivity.

Other Detectors. A wider variety of selective gas chromatographic detection devices had been described that were applicable to residue analysis, but were rarely found in typical pesticide laboratories. This might be due to the cost, complexity, or novelty of equipment or approach. A current listing might include the variety of setups utilizing emission from heteroelements in

discharges or flames (Hg, B, Sn, Pb, N, P, S, Cl, Br, I, and others), single ion monitoring by mass spectrometry, plasma chromatography, fluorescence measurements, and several more.

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COMMISSION ON HIGH TEMPERATURES AND REFRACTORY MATERIALS (II.3)

Prague, 17-18 October 1974

Present: Prof. C. B. ALCOCK (Chairman), Prof. G. D. RIECK (Secretary), Prof. E. FITZER, Prof. M. FOEX, Dr. J. HLAVÁČ, Prof. G. DE MARIA (Titular Members); Prof. F. CABANNES, Prof. P. W. GILLES, Dr. W. S. HORTON, Prof. K. MOTZFELDT, Prof. H. NOWOTNY, Dr. R. W. OHSE (Associate Members); Prof. S. MROWEC, Prof. R. SERSALE (National Representatives).

1. Minutes of Previous Meeting

The minutes of the meeting in Munich on 23-25 August 1973 (see *Comptes Rendus XXVII Conference: Part B*, pp. 155-157) were already approved by mail.

2. Reports on Sub-Committees and Task Forces

(i) *High Temperature Bibliography.* According to a report from Dr. M. G. HOCKING (September 1974), the financial status of the Bibliography had now been improved as a result of the increase of subscription. Members felt that changes in the headings might be desirable, but should only be brought about gradually. It was stressed that the addresses of authors should be added in all entries. This decision would be communicated to Dr. HOCKING. A brief statement describing the scientific activities of the Commission should be appended once a year to the Bibliography. Dr. HOCKING would be asked to send a letter to all contributors, suggesting that publicity be given in their respective national chemical journals. A possible incorporation of a data-flagging system, which was at present under consideration within IUPAC, would be considered at the next meeting.

(ii) *Carbon*. Prof. FITZER reported that British, French, and German groups had agreed to cooperate in the attempt to improve the description of various forms of carbon and graphite. The effort would include characterization and nomenclature arrived at on scientific grounds. Samples had been distributed to collaborating laboratories for comparative measurement with standard procedures. After a conference in Pittsburgh (USA) in 1975 it was hoped that USA contributions would be added. The final paper describing the cooperative study would be circulated among Members of the Commission.

(iii) *Melting Points*. After discussion of a report of an international collaborative study on Y_2O_3 submitted by Prof. FOEX, it was suggested that further studies were necessary. These would cover the effects of the oxygen pressure of the atmosphere on the melting point, resulting from changes in stoichiometry. The second point needing further study was the significance of the reaction between tungsten of the crucibles and Y_2O_3 . A letter from Prof. J. DROWART suggesting that a different statistical significance be given to the results which were presented, was considered.

Dr. OHSE would gather the information which existed on the nonstoichiometry of Group III and rare-earth oxides in relation to their melting points. Prof. NOWOTNY undertook to advise the Commission concerning possible carbide eutectic systems, which could be used for the temperature range of 2000-3000°C. Prof. CABANNES reported that further work on the ZrO_2 - $La_2Zr_2O_7$ systems had shown that this was not a suitable system.

(iv) *Data Flagging*. Dr. HORTON reported his membership of the IUPAC *ad hoc* Interdivisional Working Party on Data flagging. The second circular was being distributed to the Members, who were asked to send in their comments to Dr. HORTON with a copy to the Secretary.

(v) *Calorimetry of Vaporization*. Prof. DE MARIA reported on the microcalorimetric measurements carried out in his laboratory on the heats of sublimation of Cd, Zn, Te, SbF_3 , and BiF_3 . A high degree of accuracy could be achieved whilst the vaporization rate was being measured simultaneously.

(vi) *High Temperature X-ray Diffraction*. Prof. FOEX suggested that this study should be augmented with work using neutron diffraction. Some of his coworkers had recently carried out thermal expansion studies using the high-flux reactor at Grenoble. It was decided to ask them to extend this work with experiments on ZrO_2 , W, SiC, and graphite. Also, it was decided to drop the consideration of solid-solid transitions as temperature standards, because of hysteresis-effects in oxides. Further considerations would be given to allotropic transformation in elements, such as in Hf and Zr.

(vii) *Hot Corrosion*. Different views regarding this problem were discussed. Prof. FITZER reported that in many other organizations the problems of such corrosion were already the subject of studies. Prof. MROWEC suggested that a meeting of about 75 specialists should be convened at which should be discussed, for example, the role of shear structures, transport problems, and industrial applications. According to Prof. MOTZFELDT, no standardization would be involved in this way; however, in the more limited field of solid-gas reactions useful work might be possible. It was decided to continue the activities in another subcommittee with regard to reactions at high temperature between solids and gases (see below).

3. New Sub-Committees

(i) *Solid-Gas Reactions at High Temperatures*. The new subcommittee would

be coordinated by Prof. MROWEC and consisted further of Prof. FITZER, Prof. HLAVÁČ, Prof. MOTZFELDT, and Dr. OHSE. The goal would be to formulate steps that could be taken to characterize model systems in high temperature solid-gas reactions. The subcommittee had its first session on 18 October.

(ii) *Nonstoichiometry in Refractory Oxides*. It was felt that the defects due to nonstoichiometry played an important role in the behaviour of refractory oxides [as already stated under 2(iii)]. A new subcommittee was formed with Dr. OHSE as coordinator and Prof. ALCOCK, Prof. CABANNES, Prof. MROWEC, and Dr. B. C. H. STEELE as the other members.

4. New Task Forces

(i) *Reference Electrodes in Solid State at High Temperatures*. A note from Dr. STEELE on zirconia electrolytes would be sent to the Members. It was proposed to create a new task force in order to establish reference electrodes to be used in high temperature solid-state electrochemistry. Dr. STEELE would coordinate it with Prof. ALCOCK, other participants to be nominated by the latter.

(ii) *Optical Pyrometry*. In many high temperature processes the problem of how to measure the temperature by optical pyrometry and its accuracy was of primary importance. A new task force would clarify procedures of measuring temperatures by optical pyrometry. Prof. MOTZFELDT would coordinate it and Prof. CABANNES and Dr. HORTON would participate. A preliminary report could be ready in 1975 and for the meeting in Montpellier (see below) speakers on this subject would be invited.

5. Other Matters

(i) *Terms of Reference of Commission*. This item introduced by the Chairman and Dr. HORTON was discussed on the basis of the Byelaws of IUPAC (4.1301). Apart from the fields covered by the Commission at this moment, other activities were possible. Prof. SERSALE suggested that industry would be interested in standardization of mechanical properties in ceramics, metals, and high temperature composite materials. He would report to the Commission whether there existed already an international standardization for ceramics. Prof. MROWEC raised the question whether the Tammann temperature was the lower limit of high temperatures. Finally, 500°C was adopted as a lower limit. Prof. ALCOCK, Dr. HORTON, and Prof. RIECK would write up a proposal about the terms of reference and circulate this among the Members well before the next meeting in Madrid.

(ii) *Vocabulary for Powder Metallurgy*. Prof. RIECK reported that the International Plansee Society for Powder Metallurgy in Reutte (Tirol, Austria) had distributed free-of-charge since 1964 a vocabulary with entries in German, English, and French, and it planned a new edition. It was suggested that the Society should be asked to send a copy to each Member and each Member be requested to give individual critical suggestions to the editor. An extension to the Russian language would be recommended.

(iii) *National Representatives*. The Executive Secretary would be asked by the Chairman to write to the appropriate scientific or adhering bodies in Israel, Romania, Switzerland, USSR, and Yugoslavia, asking for a National Representative to be nominated to the Commission.

(iv) *Data for Applied Chemistry*. Prof. O. KUBASCHEWSKI had suggested by letter to the Secretary, to discuss the application of thermodynamic data. It was discussed whether computer banked data could be of help for industry. In this respect it was suggested that industry could help in the difficult financial problems in arranging meetings of the Commission.

(v) *Vaporization Standards*. Prof. GILLES was asked to look into the data of Au, Ag, and Cd and advise the Commission about further action, which was estimated to take more than 1 year.

6. Conferences

In Baden (near Vienna) in 1973 and Toronto in 1974, experts had met and discussed important items in the field of interest of the Commission. Papers from the first Conference had appeared in *Canadian Metallurgical Quarterly* [13, No. 2 (1974)] and probably the same would happen with papers from the latter meeting. Other subjects for future conferences might be: thermoconductivity, standards for calibration of high temperature apparatus, and procedures of measurements at high temperatures.

In 1975 scientific meetings would be held as follows:

(i) Montpellier (France) 25-29 August about: Thermodynamics, organized by Prof. M. LAFFITTE. It was proposed that the Chairman should try to organize on the last day a session devoted to the problems of the Commission, as a good introduction for its next meeting in Madrid.

(ii) Odeillo (France) 12-16 September about: Thermal Plasmas, organized by Dr. C. BONET.

Regarding the 28th Conference of IUPAC in Madrid, Commissions would meet during 3-6 September. Commission II.3 felt that in order to be able to have discussions in subcommittees, it would have to meet on 3rd (whole day), 4th (half day), 5th (whole day), and 6th (afternoon) of September.

G. D. RIECK

INTERDIVISIONAL COMMITTEE ON MACHINE DOCUMENTATION IN THE CHEMICAL FIELD (IDCMD)

Columbus, 17-19 October 1974

Present: Prof. J. E. DUBOIS (Chairman), Dr. D. C. VEAL (Secretary), Prof. S. FUJIWARA, Dr. H. SCHENK, Dr. C. SUHR, Dr. F. A. TATE, Dr. J. J. B. VAN EIJK VAN VOORTHUIJSEN. Dr. K. L. LOENING participated as Observer on behalf of the primary literature services, and Dr. W. H. POWELL and Dr. R. J. ROWLETT, Jr., as technical experts.

Report of Previous Meeting

A report of the meeting held in Munich on 24 and 26 August 1973 had been published in *Comptes Rendus XXVII Conference: Part B* (see pp. 90-95).

Membership

Since the last meeting Prof. FUJIWARA and Dr. VEAL had been appointed as Members, Dr. J. W. BARRETT as Observer from ICSU AB, Dr. R. N. JONES as Observer from CODATA, and Drs. L. C. CROSS, H. GRÜNEWALD, and LOENING as alternate Observers from the primary literature services.

External Relations

The Committee considered the activities of the following bodies to be potentially of interest to it: ICSU AB, CODATA, OECD, ISO, SCOPE, UNISIST, EUSIDIC. So far, little information had been collected, but the location of several of these international bodies in a joint headquarters in Paris should make liaison with them easier. A report on ICSU AB activities had been received from Dr. BARRETT, and the Secretary was asked to follow up several detailed points arising.

Standardization

The Committee noted work on data flagging being carried out by IUPAC and CODATA, and received a report on Chemical Abstracts Service (CAS) work in this area. The Committee endorsed the general concept of developing standards for data flagging, and CAS's experimental work. It was agreed to keep this area under review.

Codification

The UNISIST report 'Study on the Problems of Accessibility and Dissemination of Data for Science and Technology' was tabled. The Chairman reported that he had assisted in drafting the section on representation of chemical structure.

Machine Handling of Chemical Structures: Computer Generation of Nomenclature

The Committee received a very thorough review of CAS work in these two areas, including a tour of CAS and practical demonstrations. The Committee expressed gratitude to CAS for this review, which provided a sound basis for the ensuing technical discussions.

ICSU AB Desiderata for Chemical Nomenclature

The Committee reviewed this document, prepared by the ICSU AB Working Group in Chemistry. It was felt that it gave insufficient stress to the specific needs of index nomenclature, and that IUPAC work on nomenclature was best coordinated by IUPAC itself. These views would be conveyed to the Working Group.

IUPAC Nomenclature Commissions

The Committee felt that, to aid its work, it needed a clear picture of the current activities of the Commissions. To some extent this had been achieved by sending Observers to Commission meetings, but the Committee expressed the hope that the current changes involving the Interdivisional Committee on Nomenclature and Symbols would result in a situation in which transfer of information from, to, and between Nomenclature Commissions would be much more straightforward. Correspondence between Dr. SCHENK and Prof. N. LOZAC'H (Commission on Nomenclature of Organic Chemistry) on cyclophane nomenclature was reviewed. It was felt that there were some principles which could be invoked regarding ring nomenclature and it was agreed to review the area of phane nomenclature, as an example, in consultation with CAS.

Reports from Members

Prof. FUJIWARA reported on work being carried out in Japan on error rates in machine-readable chemical data bases and topological classification of ring systems.

Goals and Tasks of the Committee

The Committee had a long and detailed debate on this topic, based on a paper tabled by the Chairman. It was concluded that the Committee had a series of *tasks* to perform in various areas of application of computers to chemical information, *e.g.*, the machine handling of chemical structures. A logical method of approach for each task would then be to consider, in order,

- typology — classification of possibilities
- standardization — criteria for making choices from the possibilities
- codification — actual implementation of specific possibilities

The Committee's work should be essentially to lay down sound principles to govern developments in each area. It was further agreed that the Committee should concentrate on one task at a time at future meetings. It was felt this approach accorded well with the recommendations of the original Riegel report and would make the collection of papers and the organization of the Committee's work much easier.

Next Meeting

The next meeting would be held during the 28th IUPAC Conference in Madrid (September 1975). It would be a three-day meeting and would be devoted to the subject of machine interconversion of different forms of chemical structure representation.

D. C. VEAL

COMMISSION ON ANALYTICAL NOMENCLATURE (V.I)

London, 22 November 1974

Present: Prof. H. M. N. H. IRVING (Chairman), Dr. H. ZETTLER (Secretary), Prof. G. G. GUILBAULT, Dr. O. MENIS, Prof. A. J. B. ROBERTSON (Titular Members); Dr. G. F. KIRKBRIGHT, Dr. G. SVEHLA (Associate Members); Mr. R. W. FENNELL, Mr. M. J. PATER (Observers); Mr. R. J. M. RATCLIFFE (Assistant Secretary IUPAC).

Minutes of Previous Meeting

The minutes of the meeting held in Munich on 22-25 August 1973 (see *Comptes Rendus XXVII Conference*, pp. 190-192) were confirmed.

Recommendations on Usage of the Terms 'Equivalent' and 'Normal'

The Chairman welcomed Mr. PATER, representing ISO/TC 47 (Chemistry), who strongly supported the need for the retention of certain terms in general usage internationally. The letters of criticism received from GORIN, HARRIS, KRATOCHVIL, MARCUS, MEITES, PARSONS, and PLAMBECK, were discussed extensively. It was felt that further clarification of the Recommendations [Provisional Nomenclature Appendix No. 36 to IUPAC *Information Bulletin*

(August 1974)] would be appropriate and necessary. All Commission Members were requested to send their comments to the Chairman so that an amendment could be prepared. Mr. S. CUSTODERO (UNI Milano) for ISO/TC 47, should receive a copy of this draft amendment.

The question of an IUPAC representative to ISO/TC 47 for its meeting at Moscow in the Spring of 1975 was left open for further discussions with the President of the Analytical Chemistry Division.

Nomenclature of Scales of Working

According to a letter from the project leader Prof. T. S. WEST who was currently in Canada, the documents for a planned rewritten report had been lost in the mail. There were copies, however, in London and he planned to circulate the rewritten report to the Commission early in 1975 after his return to UK.

List of Synonyms and Trivial Names

A final copy of this report was turned over by the project leader Prof. IRVING to Dr. K. L. LOENING (Chemical Abstracts Service) after the Munich meeting in 1973 in order to check the names for consistency with IUPAC nomenclature in the organic field. This had not yet been completed and Prof. IRVING would write to him again.

Development and Publication of Methods of Analysis

Spectrophotometric Procedures. The question of overlap projects of the Commission on Spectrochemical and other Optical Procedures for Analysis (V.4) was still with the Division Committee. It was agreed that the approach of the two Commissions to this project was quite different and that any actual overlap could be prevented by mutual agreement.

Ion-selective Electrode Procedures. A preliminary report had been prepared and distributed by Prof. GUILBAULT. Pending further discussions, comments were invited by the project leader. The report would be distributed to all Commission Members.

Precipitation Methods. The comments of the Members present and written comments from SAMUELSON and KAISER were discussed and turned over to the project leader Dr. KIRKBRIGHT for further consideration.

Photoluminescence Procedures. The report was discussed. Written comments received from ALMGREN, SAMUELSON, and KAISER were turned over to the project leader Dr. MENIS for further consideration. The Commission was awaiting a decision from the Division Committee on what action should be taken.

Nomenclature for Liquid-liquid Distribution

A revised report (1974) was submitted by the project leader Prof. IRVING following discussion with Dr. N. M. RICE and other experts in the field. It had been made available to delegates attending the meeting of ISEC 74 in Lyon during September 1974. No comments had yet been received from them. The report would be distributed to all Commission Members for their comment. A finalized report would be presented at the Madrid meeting (1975). The Secretary was also asked to send a copy of the revised report for comment by the Commission on Electroanalytical Chemistry (V.5).

Nomenclature of Kinetic Methods of Analysis

On account of the missing documents (see above), Prof. WEST was unable to send a transcript of the discussions for a redraft which was scheduled for early 1975.

Selectivity Index

This was a longterm project and no further progress had been reported by the project leader Prof. WEST.

Criteria for Sensitivity, Detection Limits, Precision, and Accuracy

According to a recent letter from the project leader Prof. H. KAISER, the project was being worked on together with Members of Commission V.4.

Nomenclature of Data Processing

There was once again no progress to report at the present time. It was felt that some clarification of the terms of reference was necessary. A copy of the Commission V.4 Data Interpretation Report requested by Mr. FENNELL from Prof. V. A. FASSEL had not yet been received by the Commission.

Compendium of Analytical Nomenclature

The utmost urgency of this project was emphasized. Mr. FENNELL transmitted the request of the Division President to speed up any action even if other Commission projects had to be delayed in consequence of this request and the Chairman was asked to initiate an outright attack on the problems involved. Some 18 final recommendations were available for the Compendium and Mr. RATCLIFFE produced a definitive listing. After a thorough consideration of various ways of tackling the task in the light of difficulties highlighted in correspondence with FREISER and WEST, it was decided to group the documents in a rather arbitrary fashion and to submit these to separate working parties to be arranged by the Chairman, who undertook to provide close liaison with WEST and FREISER. Comparison work (test on IUPAC consistency of the terms only!) should start right away. Results should be transmitted to Prof. FREISER by 15 March 1975 at the latest, because the draft of the Compendium should be ready for submission at the Madrid meeting in 1975.

A recent letter from Prof. FREISER to the Chairman, containing a brief progress report, was considered. The existing contacts between Prof. FREISER and Dr. K. W. LOACH (Bibliographical Thesaurus of Analytical Chemistry Terms) were considered to be welcome.

Nomenclature of Photoluminescence Data

There was no further progress to report at the present time. The original draft could clearly overlap with work proposed by Commission V.4 and it was agreed that a report describing recommendations for the publication of papers dealing with photoluminescence (see above) was more in keeping with the objectives of Commission V.3.

Nomenclature of Sampling

There was no progress to report at the present time from Dr. A. C. DOCHERTY.

Information Storage and Retrieval

There was no progress to report at the present time from Prof. ROBERTSON, and it was pointed out that a substantial number of other bodies were actively engaged in this very broad field. The Division President should be asked to advise on the appropriate terms of reference and on its suitability as a project for Commission V.3.

Nomenclature of Ion-selective Electrodes

The report was discussed and written comments from DYRSSEN and KAISER were turned over to the project leader. Prof. GUILBAULT presented a redrafted final report during the meeting. He was asked to write an Introduction and pass the report to the Chairman for publication by IUPAC.

ICTA Nomenclature on Thermal Analysis

The second and third parts were under consideration and it was noted that some of the terms used were still under discussion. Further comments were required. Copies of the two reports should be distributed to all Members of the Commission for their immediate comment and the Secretary was asked to notify Dr. R. C. MACKENZIE of ICTA accordingly.

Translation of Approved English Nomenclature Texts into Russian

The Secretary was asked to notify Prof. YU A. ZOLOTOV that the Compendium (see above) was to be finalized with the greatest possible speed and that he would be informed in due course by the Secretariat when it could be translated into Russian.

Proposed Terminology and Symbol for Transfer of Solutes from One Solvent to Another

It was confirmed that Dr. RICE's letter of 21 March 1974 was to be considered as the comment of Commission V.3 regarding the proposed terminology from Commission V.5. The Division President had already received copies of that letter and of the Secretary's answer of 29 March.

Recommendations Concerning Ideal Attributes of Instruments Intended for Automated Analysis in Clinical Chemistry

The most recent version of this report from the Commission on Automation in Clinical Chemistry had been received just prior to the meeting. After discussion it was agreed that it did not concern, in general, the work of Commission V.3. However, the glossary of terms used was considered in comparison with existing IUPAC terms and no discrepancies were found. The remainder of this report, which appeared to be a collection of idealized wishes, came in for severe criticism.

Membership

It was reported that the present Titular Memberships of IRVING, BAUDIN, and ROBERTSON terminated after the Madrid meeting in 1975. Suggestions for the nomination of new Members should be passed to the Secretary.

Future Programme

The Chairman reported on proposals for the future development of the Interdivisional Committee on Nomenclature and Symbols in a new form after the Madrid meeting. The foreseeable consequences on the future activities of Commission V.3 were considered and it was noted that there appeared to be a complete lack of understanding on the unchanged and continued necessity for handling nomenclature questions within an active working group. The Chairman undertook to present these views in a letter to the appropriate IUPAC authorities.

Dr. MENIS suggested the following new projects: Nomenclature of Reflectance Measurements and Nomenclature of Standard Materials and Methods.

H. ZETTLER

MACROMOLECULAR DIVISION WORKING PARTY ON SUPPORTED POLYMER FILMS (WSPSF)

Brussels, 28-29 November 1974

Present: Mr. P. H. FINK-JENSEN (Chairman), Dr. U. ZORLL (Secretary), Mr. A. CAILLIEZ, Mr. G. CHRISTENSEN, Dr. K. M. OESTERLE, Mr. A. TOUSSAINT.

Minutes of Previous Meeting

The minutes of the meeting held at Garmisch on 15 May 1974 had been published in *Information Bulletin* No. 49 (March 1975), pp. 29-30.

Report of Chairman

As regards contacts with the Macromolecular Division (MMD), Mr. FINK-JENSEN mentioned that he had intended to participate in the MMD meeting at Madrid in September 1974, but he had received no reply to a plea for financial support. The minutes of that meeting were presented and discussed.

Efforts to promote cooperation with various professional organizations—FSPT, SLF, OCCA, and FATIPEC—had continued. A letter had been sent to Mr. L. PORTIN (SLF) regarding the possible role of WSPSF-OCS* in a future international cooperation with these organizations and their participation in WSPSF and OCS. Representatives of the four organizations met during the Atlanta convention in November 1974. Apparently the idea of ICCCI had now been abandoned and other less costly means of cooperation were being sought. A new initiative from OCS to promote international cooperation and to have the technical-scientific parts of this cooperation coordinated through the above mentioned participation in WSPSF-OCS would be appropriate.

The Chairman also mentioned that in the meantime more efforts were necessary to inform the public about the potential of the group. A certain lack of information about that could be found in nonEuropean areas. It would be worthwhile to gradually fill out this gap of information.

Membership

A new member of the group, Prof. W. FUNKE (Federal Republic of Germany), was suggested and unanimously elected; Prof. FUNKE had already expressed

* OCS—former Organic Coatings Section of Applied Chemistry Division

his willingness to participate. As decided at the previous meeting in Garmisch, Prof. R. MYERS (USA) had become a member of the group. On the suggestion of Dr. OESTERLE it was agreed that a new Swiss member should be elected. Dr. OESTERLE would proceed with this matter (Dr. THEILER of EMPA was a possibility). Mr. V. ZVONAR had approached various contacts in Eastern Europe to promote participation from that region. In particular, a possible member from German Democratic Republic was discussed and agreed to in principle. It was considered as necessary that further countries not yet represented in WSPSF should be invited to join the group in due course. An up-to-date list of members would be prepared by the Secretary, and each listed person should later confirm his membership.

Reports from Task Groups and Their Future Work

On behalf of Dr. L. A. O'NEILL, the Chairman reported about the work of the Analytical Group. The 'Recommended Methods for the Analysis of Alkyd Resins' had been reviewed in various chemical journals throughout the world. The work on acrylic resins had been wound up and publication of the results in *Journal of Paint Technology* was scheduled for February 1975 (47, 46). The corresponding results for the analysis of polyurethanes had been offered to *Journal of Oil and Colour Chemists' Association* and accepted for publication. The last item in that programme, the analysis of polyamide resins, was still under way.

The topical task of the Adhesion Group was to reformulate its objectives. It was reported by Dr. ZORLL that this should be done properly along both experimental and theoretical lines. In the future work, results of Dr. D. WAPLER about the influence of various parameters on adhesion and the quantities by which it was measured should be taken into consideration. It would also be very useful to account for the progress in instrumentation, as had become obvious from the work of the Scandinavian Paint Institute. The first task to perform would be to investigate the practical meaning, significance, and implications of the terms adherence and adhesion, so that the following work could be directed along lines useful to the surface coatings field.

Regarding Postgraduate Training, Dr. ZORLL would approach Prof. K. HAMANN, who was not present. There was a suggestion by Mr. ZVONAR, given by correspondence, also to consider individual studies in pertinent institutes, over a limited timespan, as an appropriate means of postgraduate education. Dr. OESTERLE mentioned the special item of colour measurements, on which such efforts should concentrate because of increasing use of computerized colour formulation in industry.

With respect to the progress of the Information Retrieval Group, the discussion revealed the necessity to provide material about the various information centres and their specific objectives. The Chairman would contact Mr. H. K. RAASCHOU-NIELSEN.

A thorough discussion of the Solvent-Polymer Interaction Project set up in Munich had been foreseen, but unfortunately the leader of the task group Mr. A. R. H. TAWN was unable to be present.

Discussion about Future Activities

The Analytical Group was still supposed to perform important tasks in connexion with the Solvent-Polymer Interaction Project. There might also be time for the Group to deal with one or more analytical projects, such as:

- (i) analysis of epoxy resins
- (ii) characterization of animo resins
- (iii) analysis of emulsion paints
- (iv) gel permeation chromatography

In each case a broader circle of participants than the Analytical Group itself should be aimed at.

Dr. OESTERLE had certain ideas about how the Solvent-Polymer Interaction Project should be implemented. It was decided that he should forward his suggestions to Mr. TAWN, because the Task Group was not represented at the meeting. Dr. OESTERLE proposed to investigate the advantages of the critical pigment surface concentration as a concept for paint film characterization. The effect of epitaxy with respect to polymer films would also deserve interest by WSPSF. Practical problems to be studied were felt to include all the questions encountered in printing and painting of plastics. There was a general understanding that the interaction project should illustrate both the practical and the scientific orientation of WSPSF.

To give some publicity to the WSPSF-OCS group, Mr. FINK-JENSEN suggested the possibility that the members might publish their own contributions with reference to WSPSF-OCS, which in return would assist the author with desired discussions or experimental data. This procedure might also create starting points for new activities of the Working Party. It would anyway be suitable for this purpose if articles of reports from members were disseminated within the group.

The discussion resulted in the following new proposals:

- (i) painting of plastics (TOUSSAINT)
- (ii) new methods of surface characterization (TOUSSAINT)
- (iii) interaction of paint layers (OESTERLE)

IVP put a report concerning painting on plastics at the disposal of WSPSF.

Miscellaneous

The prevailing opinion was that informal meetings of the Working Party should be arranged in connection with conventions. The next formal meeting ought to take place about November 1975, preferably in a central European location such as Stuttgart or Brussels. The Chairman would make efforts to participate in the 28th IUPAC Conference at Madrid in September 1975.

U. ZORLL

MACROMOLECULAR DIVISION WORKING PARTY ON MOLECULAR CHARACTERIZATION OF COMMERCIAL POLYMERS

Geleen, 24 January 1975

Present: Dr. BALL (Chairman), Dr. ASSIOMA, Prof. BENOÎT, Dr. BONICELLI, Dr. CONSTANTIN, Dr. HOLMSTRÖM, Dr. KONINGSVELD, Dr. MEYERINK, Dr. PRECHNER, Dr. SCHOLTE, Dr. SERVOTTE, Dr. STARCK, Dr. STRAZIELLE.

Report of Previous Meeting

A report on the meeting held at Strasbourg on 28 June 1974 had been published in *Information Bulletin* No. 49 (March 1975), pp. 30-31.

Table 1

Participant	Light Scattering		Osmometry	Viscometry		GPC	
	$M_w \times 10^{-3}$	$\langle r^2 \rangle^{\dagger}$ (Å)	$M_n \times 10^{-3}$	TCB, 135° [η] (dl/g)	$M_n^* \times 10^{-3}$	$M_w^* \times 10^{-3}$	$M_n \times 10^{-3}$
CRM (Strasbourg)	465	485	25** (α CIN, 125°)				
		435	14.7 η (α CIN, 125°)				
		485					
CdF (Mazingarbe)							
BASF (Ludwigshafen)							
ME (Novara)	750			0.77	14.6	75	120?
	770			0.90			561
	850*			0.80§	16	60	
				0.81§	16	61	
CTH (Göteborg)							
				0.88	13	68	113
				0.88*			
SNPA (Lacq)	890			0.90*	18	95	
Solvay (Brussels)	(380) \dagger	1500		0.91*			
Pekema (Kulloo)	690			0.85 \ddagger			
DSM (Geleen)	810	1400	21** (TCB, 114°)	0.84			521

*nonhomogenized Sample C (grains)

 \dagger 78% through filter

**diffusion through membrane

 η membrane SSO8§in *o*-dichlorobenzene \ddagger in TCB, 140°

Molecular Characterization of Various Polyethylene Samples

1. After being modified on some minor points, Dr. STRAZIELLE's manuscript dealing with the characterization of an HDPE polymer (homogenized Eltex 6009) and its fractions, and an LDPE polymer (homogenized Sample B) and its fractions, was approved for publication in the IUPAC journal *Pure and Applied Chemistry* [scheduled Vol. 42, No. 4 (1975)].

2. The reports of the participants concerning characterization of the homogenized sample LDPE C, distributed in October 1974, were considered. This characterization had concerned the following determinations:

light scattering	— M_w and radius of gyration $\langle r^2 \rangle^{\frac{1}{2}}$
osmometry	— M_n
viscometry	— $[\eta]$ in 1,2,4-trichlorobenzene at 135°
gas phase	— M_n^* and M_w^* (calculated with linear calibration)
chromatography	M_n and M_w

Table 1 gave a survey of the data found by the various research groups.

Light Scattering. All participants used α ClN as the solvent; temperature 125-140°. Solvay filtered through a glassfilter with bentonite as filter-aid; 22% of the sample remained on the filter (adsorbed on the bentonite). CRM also filtered through glass. SNPA and Pekema did not use a stabilizer. CRM performed tests with and without application of an antioxidant, no differences were found between the results.

Osmometry. The M_n -values 25×10^3 (CRM) and 21×10^3 (DSM) were too high owing to diffusion of the lowest molecular weight part of the sample through the membrane.

Viscometry. ME found that the $[\eta]$ -value of the sample in solution decreased with time from 0.80 to 0.76 dl/g.

Gas Phase Chromatography. For the examination of LDPE, BASF used special calibration curves determined on fractions of LDPE. The elution volume of the peak was correlated (although not quite correctly) with the M_w of the fraction determined with light scattering. The calibration curves for three LDPE's of different density were determined by measuring three series of fractions made from these polymers. Applied to an LDPE sample, the calibration curve corresponding to the relevant density yields the right MWD, M_n and M_w . At CTH, the GPC (styragel) was calibrated with narrow polystyrene samples as well as with polyethylene samples. The calibration curve was checked with NMWD-HDPE and BMWD-HDPE. Application of the linear calibration curve yielded M_n^* and M_w^* . M_n and M_w were determined with the Drott-Mendelson method (with $b = \frac{1}{2}$).

Degradation of Sample. Dr. HOLMSTRÖM suspected his sample to be partially degraded (as powder, without stabilizer) before the measurement. Dr. SERVOTTE found 22% of his sample adsorbed to the benzonite during filtration. He further noted, both with homogenized sample B and with homogenized sample C, partial adsorption of the polyethylene in the spherasil columns during GPC (adsorption of the lightly oxidized polyethylene to the glass?). In the tests with other LDPE samples (*i.e.*, the original sample B) no polymer stayed behind, neither during filtration nor during the passage through the spherasil columns. This adsorption might account for the low M_w -values from light scattering (CRM, Solvay).

Mark-Houwink Relation. Some values used for the Mark-Houwink relation $[\eta]=K.M^a$ of linear polyethylene in 1,2,4-trichlorobenzene at 135°C were given in Table 2.

Table 2

	Range	K	a
DSM*	$10^4-2 \times 10^6$	3.01×10^{-4}	0.75
NBS	$2 \times 10^4-6 \times 10^5$	4.2×10^{-4}	0.723
SNPA	$2 \times 10^3-7 \times 10^5$	7.2×10^{-4}	0.675
Solvay		5.1×10^{-4}	0.706

*Values corrected for the width of distribution.

3. Influence of peak broadening on the determination of MWD and $g'(M)$ by combined GPC and $[\eta]$ -determination of gas phase chromatographic fractions. GPC yielded the elution volume V_e , from which, by means of universal calibration $[\eta]M$ could be determined for each GPC-fraction of a branched polymer. Using a viscometer one could also determine $\Delta\eta$ ($=\eta-\eta_{\text{solvent}}$) for each fraction, and from this and c the intrinsic viscosity $[\eta]$ could be calculated. The quantities $[\eta]M$ and $[\eta]$ gave M for each fraction and, hence, the molecular weight distribution. For each fraction M and $[\eta]$ also gave $g'=[\eta]/[\eta]_{\text{lin}}$ ($[\eta]_{\text{lin}}=KM^a$).

If peak broadening occurred, the above procedure led to wrong results. For any elution volume on the low molecular weight side of the curve, M was too high owing to diffusion. Hence, using the universal calibration, one found too low a value for $M[\eta]$. On the high molecular weight side of the curve the situation was just the reverse; here one calculated too high a value for $M[\eta]$. One might say, therefore, that:

- (i) Application of the correct $[\eta]$ -value gave too broad an MWD.
- (ii) The M -value calculated on the low molecular weight side was too low, with the result that too high a value was found to $g'=[\eta]/[\eta]_{\text{lin}}$. This calculation could easily yield a g' -value greater than 1 on the low molecular weight side. On the high molecular weight side one calculated too low a value for g' .

Prof. BENOÎT gave a short survey of a method, developed at his laboratory by L. MARAIS, by means of which a correction could be made for this diffusion effect. It started from two assumptions:

- (i) The calibration curve was linear $V_e=a \log M+b$.
- (ii) Each molecular weight spread around its 'ideal' elution volume according to a Gaussian distribution $c=c_0 \exp. \left\{ \frac{-(V-V_e)^2}{2\sigma^2} \right\}$

The calculations yielded the average molecular weights of each GPC fraction expressed in terms of M_e , i.e., the molecular weight corresponding to the elution volume of that fraction:

$$\frac{\sigma^2}{a^2} = \tau^2 \quad c' = \frac{\delta c}{\delta \log M}$$

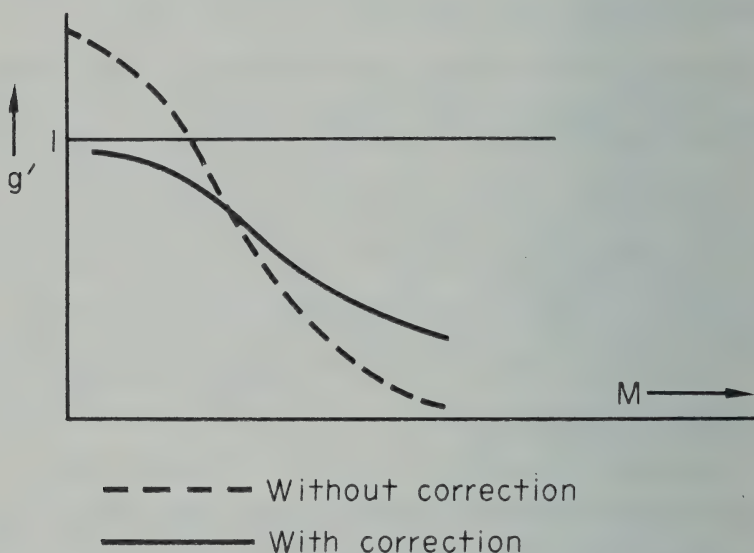
$$M_w = M_e \exp. \frac{3}{2} \tau^2 \left[1 + \tau^2 \frac{c'}{c} + \tau^4 (c'', c''') \dots \right]$$

$$M_n = M_e \exp. \frac{1}{2} \tau^2 \left[1 + \tau^2 \frac{c'}{c} + \tau^4 (c'', c''') \dots \right]$$

$$M\eta = M_e \exp. \frac{\sigma+2}{2} \tau^2 \left[1 + \tau^2 \alpha \frac{c'}{c} + \tau^4 (\quad) \dots \right]$$

$$\frac{M_w}{M_n} = \exp. \tau^2 \left[1 + \tau^4 \left(\frac{c''}{c} - \frac{(c')^2}{c^2} \right) \dots \right]$$

In experiments with some synthetic rubbers, MARAIS indeed found that this correction led to a good $g' = f(M)$ relation.



It was necessary to determine σ as a function of V_e . The value of σ depended on the packing material and had an almost constant value in the middle part of the range of elution volumes. With spherosil it was much greater than with styrogel.

Future Programme

Before the next meeting, two samples of LDPE (Stamylan 1500 and Stamylan 1523 S) would be characterized:

$[\eta]$ in TCB, 135°

M_w by light scattering

M_n by osmometry

GPC: M_n^* , M_w^* , $M_n^{*'}$

M_n M_w M_z

g' as a function of M

IR (by BASF and DSM)

NMR (by Solvay and DSM)

100 g of each sample would be sent to the participants.

The next meeting would be held in the office of CdF 'Tour Aurore' in Paris La Défense on 28 November 1975.

H. BENOÎT

COMMISSION ON TOXICOLOGY IN CLINICAL CHEMISTRY (CT_oCC)

London, 19-20 February 1975

Present: Prof. F. W. SUNDERMAN, Jr. (Chairman), Prof. R. BOURDON (Secretary), Dr. S. S. BROWN (Titular Members); Dr. J. SAVORY, Dr. D. B. TONKS (Associate Members); Dr. A. CERNIK, Dr. K. F. LAUER, Dr. L. MORGAN, Dr. M. P. H. SAYERS, Dr. A. SMITH (Observers); R. J. M. RATCLIFFE (Assistant Secretary IUPAC).

Minutes of Previous Meeting

The minutes of the meeting held at Munich on 19-20 April 1974 were approved [see *Information Bulletin* No. 48 (October 1974), pp. 37-38].

International Symposium on Metals

1. Unanimous approval was recorded of the mail vote (a) to change the title of the forthcoming meeting to 'International Symposium on Clinical Chemistry and Chemical Toxicology of Metals', (b) to schedule the Symposium in September-October 1976, and (c) to adopt the revised format of the scientific programme.
2. A statement on 'Goals and Scope' of the Symposium was drafted, revised, discussed, and adopted unanimously for inclusion in the Preliminary Announcement.
3. A statement on 'Organization of the Symposium' was drafted, revised, discussed, and adopted unanimously for inclusion in the Preliminary Announcement.
4. A report by Mr. RATCLIFFE on possible meeting sites was discussed. Tentative agreement was reached to hold the meeting in Western Europe (probably at Monte Carlo), because the hotels there would provide gratis meeting and exhibition facilities, and the government would provide attractive inducements, such as a gratis reception. Prof. BOURDON and Mr. RATCLIFFE agreed to investigate hotels and dates, and to present a formal recommendation at the next meeting.
5. A preliminary budget for the Symposium was drafted by Dr. TONKS, revised, discussed, and adopted unanimously.
6. Mr. RATCLIFFE suggested that Trans World Conference Organisers Ltd. be selected as the official agent to assist in administration of the Symposium. This proposal was tabled until the next meeting, pending receipt of a detailed statement regarding the services to be rendered and the financial arrangements (particularly covering the responsibilities for any debts which might be incurred by the Symposium in excess of receipts).
7. Dr. BROWN agreed to serve as (a) Secretary of the Symposium Committee, and (b) Editor of the Proceedings of the Symposium. After extensive dis-

cussion, it was decided that the proceedings would best be published either as a separate book or as a special issue of an appropriate journal. Dr. BROWN would request the IUPAC Executive Committee to waive the publication rights of the Union. He could then explore possible publishers and present a recommendation at the next meeting.

8. The Preliminary Announcement (First Circular) would be mailed immediately after the next meeting, assuming that the location, hotel, dates, and financial arrangements were approved. It was anticipated that 15,000 copies of the First Circular would be mailed, with primary responsibilities assigned to Prof. M. MERCIER (Western Europe), Dr. BROWN (UK), Prof. SUNDERMAN (USA), and Dr. TONKS (Canada).

9. The possibility of arranging for commercial exhibits at the Symposium was assigned to Dr. H. E. SPIEGEL and Dr. SAVORY for investigation. Their recommendations would be anticipated at the next meeting.

10. Extensive discussion was given to the Scientific Programme of the Symposium, and to a potential list of plenary lecturers. Prof. SUNDERMAN's draft programme was revised and adopted.

11. Drs. SAYERS, CERNIK, and SMITH of the Health and Safety Executive (UK) discussed the British programme for quality control of blood lead analyses, and proposed that such interlaboratory standardization of metal analyses be a major topic of the Symposium. This proposal was adopted enthusiastically.

12. Dr. LAUER (Belgium) of the CEE Directorate-General for Research, Science, and Education, described the manifold activities of the Commission in the sphere of toxicology and outlined its possible interest in cosponsorship of the Symposium.

Other Business

Section on Air Quality. Dr. BROWN and Prof. BOURDON reported on their attendance at the meetings of the IUPAC Section on Air Quality in Paris [25-27 September 1974: see *Inf. Bull.* No. 49 (March 1975), pp. 71-74]. The Commission on Toxicology unanimously approved their suggestion that the Commission should offer its help and assistance to the Section in any endeavour which might relate to measurements of toxic agents in body fluids, tissues, or excreta.

Inter-Union Symposium on Mechanism of Drugs. Information on this proposed joint symposium with IUPHAR would be distributed to Members of the Commission on Toxicology.

26th IUPAC Congress (Tokyo, September 1977). The Commission on Toxicology would offer to participate in the Joint Symposia on 'Chemistry and Welfare of the Human Being'. In particular, this might be the appropriate time for a 'Symposium on Gas Chromatography/Mass Spectrometry of Drugs and Toxic Agents in Body Fluids'.

Date and Place of Next Meeting

The next meeting of the Commission would be held in conjunction with the IX International Congress of Clinical Chemistry at Toronto in July 1975.

F. W. SUNDERMAN

COORDINATING COMMITTEE FOR ANALYTICAL METHODS FOR CEE AND IARC

Birmingham, 9 May 1975

Present: Prof. R. TRUHAUT (Chairman), Prof. F. PELLERIN (Secretary), Prof. R. BELCHER, Dr. H. EGAN, Dr. R. MARCUSE.

Minutes of Previous Meeting

The minutes of the meeting at The Hague on 30 July 1974 [see *Inf. Bull.* No. 49 (March 1975), pp. 79-81] were approved, noting that it was a meeting of the Liaison Group rather than of the full Coordinating Committee. The present meeting was only of the Liaison Group.

Information from Chairman

The Chairman gave an account of the present state of IUPAC-CEE relations concerning the longterm execution of the cooperative programme aiming to establish analytical methods for the control of purity standards of additives in food.

He mentioned the reasons why CEE had to stop the further development of contracts arranged annually since 1967. CEE had not yet been able to summon its intergovernmental experts to the foreseen meeting with representatives of IUPAC. Moreover, CEE had not directed the methods to its experts gradually during the execution of each contract. This had resulted in an accumulation of a considerable number of methods which remained to be examined and discussed by CEE. On the other hand, the positive list of emulsifiers and stabilizers for food usage following those of colorants, antimicrobials, and antioxidants, had certainly been established. However, in that case, it remained to fix the purity standards, a knowledge of which conditioned the establishment of analytical methods for their control. Therefore it was necessary to expect that this work, which was incumbent on CEE, should have been effected.

Prof. TRUHAUT reported that, in accordance with the instructions of the IUPAC Executive Committee, he had made contact with the CEE authorities to find out the future programme of IUPAC-CEE cooperation. He sent a report on this subject to the Secretary General, Dr. GALLAY, who submitted it to the meeting of the Executive Committee held in Moscow at the end of February 1975. At that meeting, it was decided the President of IUPAC should go to Brussels with Prof. TRUHAUT to discuss the future programme of scientific cooperation between IUPAC and CEE. The date of the meeting had now been fixed for 6 June 1975.

Dr. EGAN intervened to emphasize a certain number of points already mentioned in the activity reports of the Coordinating Committee presented by its Chairman to the Bureau and to which the attention of the CEE authorities had already been drawn on several occasions:

- (i) It appeared that certain purity standards did not correspond to present manufacturing conditions or synthesis of some of the additives (*e.g.*, organically bound chlorine in benzoic acid and its salts, salicylic acid in *p*-hydroxybenzoic esters and their sodium derivatives). There would be major interest if one of the future contracts concerned the specification of adequate purity standards taking into account technological changes in industrial chemistry.
- (ii) Certain methods sent to CEE in execution of contracts since 1967 were

now obsolete, by reason of refining of analytical techniques and improvement of sensitivity and specific features of methods.

(iii) He emphasized the necessity for an effective link between the two organizations, that is to say groups of intergovernmental experts of CEE and experts of IUPAC. The remarks and suggestions presented by the former would thus be able to be communicated to the latter with a view to their taking them into account and formulating a reply.

On this subject the Chairman recalled his repeated demands for a IUPAC representative to be present at the meetings of intergovernmental experts of CEE in order to reply to their questions and possibly their criticisms. Unfortunately CEE, being given its heavy tasks, had not been able so far to effect this wish. During his recent conversations with the CEE authorities, the Chairman again insisted on the importance attached to practical realization of mixed meetings.

Methods still Outstanding

Prof. PELLERIN reported that 5 methods could not be sent to CEE with the other methods of the 1974 Contract, because of reservations made by certain Members from either the Commission on Analytical Reactions and Reagents or the Food Section. It was pointed out to the CEE authorities that these methods would be sent as soon as relevant problems were resolved.

Method 3/74 (Sulfur trioxide in sulfur dioxide). Prof. BELCHER indicated that a method was being studied in his laboratory, based on flame spectrometry, which allowed a quick and specific determination. A demonstration of the method was given to the Members present by Prof. BELCHER and his colleague Dr. S. L. BOGDANSKI. This method would shortly be published and put into a form to satisfy the CEE requirements. As soon as it was written up, the Secretary would get it circulated, according to normal custom, for definite adoption at the meeting in Madrid later in the year.

Methods 4-5/74 (Determination of organically bound chlorine in benzoic acid and benzoates). The method had given rise to a wide exchange of views. It was decided to send to CEE the method for determination of total chlorine which had been proposed originally by Dr. P. L. SCHULLER. This should be accompanied by comments emphasizing the following points:

(i) The method was no longer adapted to control of the purity of benzoic acid and its salts, from the fact of evolution of the techniques of industrial synthesis which involved the oxidation of toluene.

(ii) The limits figuring in the CEE's directive were too lax.

(iii) Taking into account present evolution, it was up to CEE to fix limits for inorganic chlorine and for organically bound chlorine. When CEE had brought its limits up to date and provided more useful guides, IUPAC would be in a position to introduce a new method better adapted to the present situation.

Method 9/74 (Nonvolatile matter in sulfur dioxide). During the session, Dr. EGAN had written a note which received the approval of Members present. It would be communicated to Dr. SCHULLER for approval, then it would be sent to CEE. Dr. MARCUSE agreed to undertake an enquiry into the service of manufacturers with a view to collecting information on methods of analytical control of sulfur dioxide.

Method 10/74 (Nitrites in potassium nitrate). The method had already been sent to CEE in advance for the 1974 Contract. Therefore it was a mistake that it was mentioned as not having been provided for CEE. To avoid any misunderstanding, a copy of the method would be attached when the other outstanding methods were finally sent.

Remarks from Dr. Schuller (letter of 74.11.27:
US17/74:LCLO/SCH/ne)

The difficulties encountered by Dr. SCHULLER in dissolution of sodium derivatives of *p*-hydroxybenzoic esters were apparently connected with the fact that the appearance of commercial samples was often very different; sometimes they did not show a crystalline appearance and the quickness of dissolving was then affected. Prof. PELLERIN also recalled that the sodium derivatives of these esters were not very stable and underwent a very rapid saponification in the presence of humidity or in solution.

The Liaison Group, taking into account the reservations of Dr. SCHULLER, decided to change the last two lines of the English text of Method 8/74:

instead of 'Before the dilution to 50 ml, the mixture is acidified to litmus paper with 2N sulphuric acid'

write 'pH is adjusted to 5 before the dilution to 50 ml'.

Because the method had already been sent to CEE, a correction would be communicated at the time of revision.

Atomic Absorption

The Chairman recalled that at the meeting in Paris on 10 April 1973, Dr. MARCUSE accepted the task of undertaking research on the application of atomic absorption to the detection and determination of mercury, lead, copper, and cadmium in food additives (antimicrobials, antioxidants, colorants). Dr. MARCUSE pointed out that there was a misunderstanding. The research had been undertaken for the determination of these metals in food (and not in additives for food). Research had been followed up in this sense by Dr. K. KOJIMA, Chairman of the Food Contaminants Commission. Prof. TRUHAUT emphasized the interest in this problem, which involved mineralization difficulties in the case of food; in the case of additives, the problem should be resolved more easily. He asked Dr. MARCUSE to pay special attention to the detection of mercury in additives and to inform Dr. KOJIMA of the importance of this research also in the case of additives.

Prof. PELLERIN pointed out that one of his students (Mr. J. P. GOULLE) would present a thesis in June 1975 on the detection of traces of lead, copper, zinc, and cadmium in various organic compounds, notably colorants and other additives; these methods were the subject of a short communication to the Académie de Pharmacie de Paris. He proposed to prepare the text of methods so developed, with a view to circulation according to usual sequence ready for discussion at Madrid in September 1975.

Methods of Rapid Analysis

Prof. TRUHAUT thanked Dr. MARCUSE for his proposal (letter of 74.12.13). After an exchange of views, it appeared that in the framework of IUPAC-CEE contracts, IUPAC's activity could not be materialized by sending to the CEE authorities methods of this type which were still in the exploration stage. This opinion had also been formulated by Dr. SCHULLER (letter of 75.4.28).

Miscellaneous Matters

In preparation for the Brussels meeting on 6 June 1975, Prof. PELLERIN proposed to prepare a note mentioning the various points outstanding which called for replies from CEE.

With respect to the Standing Orders for the Coordinating Committee approved at the recent Moscow meeting of the Executive Committee Prof. TRUHAUT recalled that in October 1975 he would have fulfilled his Office as Chairman of the Coordinating Committee for 8 years. Dr. EGAN suggested that in the present situation of the cooperative programme with CEE and taking into account that this programme introduced important toxicological aspects, it was desirable that an exceptional prolongation of 2 years be granted to Prof. TRUHAUT until October 1977. Dr. EGAN considered that it would be desirable not to limit the task of the Coordinating Committee to the cooperative programmes with CEE and IARC, but to extend it to the realization of programmes with other organizations such as FAO, WHO, and UNEP.

MACROMOLECULAR DIVISION WORKING PARTY ON STRUCTURE AND PROPERTIES OF COMMERCIAL POLYMERS

Paris, 19-20 June 1975

Present: Dr. A. J. DE VRIES (Chairman), Dr. M. E. CARREGA (Secretary), Dr. G. AJROLDI, Dr. G. G. A. BÖHM, Mr. C. BONNEBAT, Dr. J. CHAUFFOUREAUX, Dr. P. L. CLEGG, Dr. M. FLEISSNER, Dr. GARCIA-ESTARTUS, Mr. A. GHIJSELS, Dr. P. J. LAURIJSEN, Prof. A. S. LODGE, Prof. J. MEISSNER, Dr. H. MÜNSTEDT, Dr. H. H. MEYER, Dr. A. K. VAN DER VEGT, Mr. J. L. S. WALES.

Minutes of Previous Meeting

The minutes of the meeting held at Ludwigshafen on 28-29 November 1974 [see *Inf. Bull.* No. 49 (March 1975), pp. 78-83] were approved.

The final report by Dr. T. T. JONES on the Polystyrene programme had been accepted for early publication in *Pure and Applied Chemistry* during 1976 (scheduled Vol. 45 No. 1). The final report on the PVC Rheology programme written by Mr. J. L. S. WALES was to be published in a special issue of *J. Polymer. Sci. (Part C)* devoted to the proceedings of the 1974 Madrid International Symposium on Macromolecules.

Members participating in the HIPS programme were reminded that final results were to be sent to Dr. W. RETTING before 1 July 1975. Dr. CHAUFFOUREAUX had distributed the final report on the first part of the programme on tensile properties of rigid PVC. Members were requested to send their comments before 1 September in order to enable the Chairman to submit this report for publication as soon as possible. Members were also reminded to send to Dr. CHAUFFOUREAUX the results on the second part of the programme on PVC (effect of fillers) before 15 October 1975.

With regard to the report presented by COLLINS and NAKAJIMA at the Society of Rheology meeting in October 1974, the Working Party considered that this report did not provide sufficiently new information to warrant publication separate from the final report by WALES which would be published soon in *J. Polymer Sci.* As to the presentation of the complete final

report at the forthcoming Society of Rheology meeting in St. Louis (Miss.) in October 1975, as proposed by COLLINS and NAKAJIMA, the Working Party did not reply positively to this proposal because the report was already presented at an International Meeting (IUPAC Symposium in Madrid, 1974) and would be published soon. DE VRIES would inform COLLINS on these decisions of the Working Party.

Rheology of Block Copolymers

The first progress report on this programme was presented by Mr. GHIJSELS and discussed extensively. The results of the different laboratories were in fair agreement, in particular with regard to capillary rheometry, but significant discrepancies between the results of different laboratories were observed in cone-and-plate flow. Following a proposal by Prof. LODGE, it was decided to study in detail the time dependence of shear stress at constant shear rate in cone-and-plate flow. The following experimental conditions were agreed upon:

two shear rates: 0.01 and 0.1 s^{-1}

temperature: 150°C

cone angle: 2°

samples to be prepared by compression-moulding at 150°C for 10 min and a pressure of 0.7 MPa (100 psi) and quickly cooled (5 min under pressure).

After detailed discussion of the possible importance of heating time and geometry of the mould, it was finally decided to request each member laboratory to use its own method but to keep a record of all experimental details. With respect to some peculiar and unexpected results of normal force measurements in cone-and-plate flow, it was agreed that it would be useful to try to obtain direct information on structural changes by means of electron microscopy. Dr. BÖHM presented some preliminary results of electron microscopy studies by Firestone.

Dr. MÜNSTEDT reported on tensile viscosity measurements in creep flow at constant stress at 130°C . At relatively low tensile stresses Hencky-strain became a linear function of time, the corresponding tensile viscosity being about three times as high as the shear viscosity. The specimens used were strands extruded at very low flow rate. Dr. CLEGG also presented tensile viscosity data calculated from convergent flow analysis by COGSWELL. The latter results obtained at 150°C showed that, in general, the ratio between tensile- and shear-viscosity seemed to be much higher than 3.

It appeared from the general discussion concerning all results obtained so far, that some of the rheological phenomena observed might be explained in terms of more or less reversible structure breakdown dependent on the magnitude of stress, strain amplitude, and deformation rate or frequency. Besides the need for direct observations by means of electron microscopy, more detailed information on the following points seemed to be particularly useful:

time dependence of shear- and normal-stresses in shear flow

effect of change of sign of shear rate on the measured values of viscosity (difference between measurements at increasing or decreasing values of shear rate, respectively)

effect of waiting time (annealing) in shear and elongational flow

effect of frequency and strain amplitude on dynamic viscosity

It was expected that the results of such a programme would allow one to determine to what extent the observed rheological behaviour was really affected by the specific domain structure of this block copolymer. Only after completion of this first experimental programme on Cariflex TR-1102, might an extension to other block copolymers be considered and a suitable choice be made.

In order to enable Dr. VAN DER VEGT and Mr. GHIJSELS to prepare carefully the final report, which would be discussed at the August meeting in 1976, all participating Members were requested to issue their results before 25 December 1975.

Results Obtained in Past Rheology Programme on LDPE and PVC

The final report on the extensive programme on three similar LDPE-samples supplied by BASF, would be published shortly in *Pure and Applied Chemistry* [scheduled Vol. 42, No. 4 (1975)]. A summary of the report, to be submitted for publication in various specialized polymer journals, was presented by Prof. MEISSNER. One of the remarkable results, as emphasized by Prof. LODGE, was the difference found in normal stress behaviour for samples exhibiting identical flow curves. Present molecular theories did not seem able to explain such differences in a satisfactory manner. Prof. LODGE's network theory was found to be rather successful in explaining the behaviour in elongation, at least qualitatively, but seemed to require some modification of its basic assumptions if quantitative agreement between theory and experiment was to be attained. From the experimental point of view, he observed that in cone-and-plate flow at higher shear rates, shear might not be homogeneous across the gap and that experimental results should be considered, therefore, with circumspection. The importance of response time and its dependence on cone angle was also mentioned.

Although it was generally agreed that the LDPE rheology programme had been particularly important for the development and improvement of experimental methods in nonlinear viscoelasticity of polymer melts, it was also obvious from the discussion that no general agreement prevailed concerning the relevance of the numerous results collected in the course of this programme to the practical industrial problems of LDPE processing and end-use performance. Several Members emphasized the importance of crystallization kinetics and its interference with purely rheological phenomena in the film blowing process and suggested that detailed experimental investigations in this field would be required for a better understanding of the differences in behaviour observed in industrial practice.

A new programme on LDPE might be envisaged and would probably interest a sufficient number of Members if no other proposals were considered more worthwhile as an object of study for the Working Party. Prof. LODGE would contact Union Carbide, who might be interested in participating in a new programme on LDPE.

Mr. WALES summarized the results of the PVC-rheology programme, which had been presented at the 1974 Madrid Symposium. One of the problems often discussed with regard to PVC-rheology, the occurrence of 'slip' at the wall, had been studied in considerable detail in the course of the programme. No conclusive evidence for slip was found at temperatures higher than 180°C. At lower temperatures slip might occur as well as structural changes in the melt, but more work would be necessary in order to understand some of the

apparently contradictory findings and to obtain direct evidence for the existence of a particulate structure. Extrudate swell and other effects of melt elasticity would also merit a more detailed study by the Working Party.

Proposals for New Programmes

An extensive list of possible future topics (11 items) for cooperative investigation was presented by ICI; a proposal for a new programme on PVC rheology was sent in by B. F. GOODRICH. Following a proposal by Dr. CLEGG it was decided to postpone any detailed discussion of new programmes until all Members had prepared a list of possible topics suitable for cooperative investigation. As had been pointed out by Dr. CLEGG in a letter to the Chairman (February 1975), sufficient time should be spent during the meetings of the Working Party in detailed planning of programmes after a reasonable choice had been made of those topics most liable to provide usable information for the polymer industry as well as presenting a scientific interest.

All Members were requested to send their list of possible future topics to the Secretary before 1 September 1975. At the next meeting(s) an attempt would be made to rank the various proposed topics in accordance with their priority before making a final choice.

Membership

Dr. H. H. WINTER (Head of the Rheology Department of IKT, University of Stuttgart), who was particularly interested in the relationship between polymer melt rheology and processing behaviour, had applied for active membership. His laboratory had started an investigation of the SBS-copolymer supplied by Shell, with the aid of a slit viscometer, without obtaining any publishable results until now. It was agreed that Dr. WINTER would be an acceptable Member, in particular if his laboratory was able to make a substantial contribution in the field of polymer processing, as suggested by Prof. LODGE. Du Pont de Nemours (Elastomer Chemicals Department, Wilmington) had not yet definitely decided on its possible active membership.

It was observed by the Chairman that specialization of the meetings, rheology and processing on the one hand, and mechanical behaviour and end-use properties on the other hand, had practically no effect on the number of Members attending. Because a critical size for effective work had now been attained, the Working Party should become more selective in accepting new Members and insist that actual Members, no longer active, resigned from membership. The Members present invited the Chairman to take the necessary steps in order to find a satisfactory solution to this problem.

Date and Place of Next Meetings

The next meeting, to be devoted to the programmes on mechanical properties of PVC and HIPS, was decided to be held on 27 and 28 November 1975. The Chairman would ask Monsanto Ltd. to organize the meeting, either in London or another appropriate place. The following meeting, devoted to rheology, would be held in Amsterdam on 19 and 20 August 1976.

M. CARREGA

COMMISSION ON TOXICOLOGY IN CLINICAL CHEMISTRY (CToCC)

Toronto, 16 July 1975

Present: Prof. W. SUNDERMAN, Jr. (Chairman), Prof. R. BOURDON (Secretary), Dr. S. S. BROWN (Titular Members); Dr. J. SAVORY, Dr. H. E. SPIEGEL, Dr. D. B. TONKS (Associate Members); Prof. P. LOUS, Dr. M. ROTH (Observers).

Minutes of Previous Meeting

The minutes of the meeting held at London on 19-20 February 1975 [see *Inf. Bull.* Nos. 50/51 (November 1975), pp. 119-120] were adopted.

International Symposium on Metals

Location and Accommodations. Prof. BOURDON and Dr. BROWN reported on their recent site visit to Monte Carlo in order to assess its suitability as the site. After lengthy discussion of possible alternative sites for the Symposium, Monaco was selected as the best site.

Dates. Prof. SUNDERMAN reported on communications to the Commission on Toxicology from Prof. M. RUBIN (President of IFCC) which expressed some concern that an International Symposium on Metals held in Monte Carlo in September-October 1976 near the time of the European Congress in Prague might tend to detract from the attendance at the latter meeting. In order to avoid any possible conflict with the IFCC meeting and after extensive discussions of other possible conflicting meetings in Europe and North America, it was decided to reschedule the Symposium for early March 1977 (3 days within the period from 1 to 12 March).

Publication of Symposium Proceedings. Dr. BROWN reported on his discussions and correspondence with numerous scientific journals and publishers regarding the publication of the proceedings. *Clinical Chemistry* (the USA journal) had expressed willingness to publish the proceedings as a special issue, and two publishers (Pergamon Press and Oxford University Press) were willing to publish the proceedings as a hard-cover book. Dr. BROWN indicated that it would be possible to publish a book within 4 months after receipt of manuscript, at a cost of approximately \$20 (US), provided the book contained the full text of the plenary lectures and abstracts (1-2 pages) of the contributed papers.

Financial Aspects. Dr. TONKS proposed a revised budget for the Symposium, based on additional data obtained since the previous meeting. Each item was discussed in detail, after which the revised budget was adopted.

Possible IFCC Sponsorship. Prof. SUNDERMAN reported that Prof. RUBIN had indicated informally that IFCC might be willing to serve as a cosponsor of the Symposium. After discussion, Prof. SUNDERMAN was authorized to invite IFCC to serve as a cosponsor.

Exhibits. Dr. SPIEGEL reported on the plans for commercial exhibits. He proposed that the exhibitors be limited to concerns that had products of particular relevance to the topic of the Symposium.

By limiting the commercial exhibits in this way, Dr. SPIEGEL anticipated that the scientific contribution of the exhibit would be greatly enhanced.

Preliminary Circular. Dr. BROWN reported on plans for the Preliminary Announcement Circular for the Symposium.

The Circular should be ready for review by the Commission at the Madrid meeting in September and 15,000 copies should be ready for mailing in late September or early October 1975.

Other Business

Relationships with WHO. Prof. BOURDON reported on his attendance as official representative of IUPAC at the meeting of the WHO Task Group on Environmental Health Criteria for Lead (Geneva, 29 April-5 May, 1975).

Prof. SUNDERMAN reported on correspondence from the Executive Secretary of IUPAC, inviting the Commission on Toxicology to review and comment upon WHO Environmental Health Criteria Documents. He had personally reviewed the first criteria document on manganese and had agreed to review certain additional documents. The Commission expressed its desire to participate actively in assisting WHO in reviewing these documents, which would have far-reaching implications in environmental toxicology.

IUPAC Organizational Matters. Dr. TONKS reported on the relationships between the Commission on Toxicology in Clinical Chemistry and the Section on Air Quality of the Applied Chemistry Division. After considerable discussion, it was decided unanimously that the Commission on Toxicology considered the measurement of all toxic agents in biological samples to be within its scope of interest and activities, regardless of whether or not the measurements were automated or were currently performed in many hospital laboratories. Prof. SUNDERMAN agreed to contact the Section on Air Quality during the Madrid Conference of IUPAC in order to attempt to resolve jurisdictional matters and to establish a harmonious and cooperative relationship.

Madrid Meeting Plans. Prof. SUNDERMAN announced that the next formal meeting of the Commission on Toxicology would be held in Madrid on 4-6 September 1975 during the 28th IUPAC Conference.

London Meeting Plans. Dr. BROWN reported that he planned to contact the CIBA Foundation in London in order hopefully to arrange for a meeting of the Commission on Toxicology in June 1976, in order to plan the details of the scientific programme of the International Symposium on Metals and in order to begin to plan for the proposed Symposium on Gas Chromatography/Mass Spectrometry of Drugs and Toxic Agents in Body Fluids, which the Commission on Toxicology hoped to present as part of the Joint Symposia on 'Chemistry and Welfare of the Human Being' at the 26th IUPAC Congress in Tokyo (September 1977).

Additional Activities. Dr. TONKS discussed possible additional activities that the Commission on Toxicology might consider undertaking, such as the development of certain reference methods. Dr. ROTH suggested that formulating criteria for specimen collection in trace metal analyses might be a valuable task. No action was taken on these matters, which were postponed for discussion at the Madrid meeting.

F. W. SUNDERMAN

REPORTS OF IUPAC-SPONSORED SYMPOSIA

IV INTERNATIONAL CONFERENCE ON CRYSTAL GROWTH

Tokyo, 24-29 March 1974

ICCG-4 was held at the Palace Hotel and Keidanren Kaikan in Tokyo. The number of participants was 776 from 22 countries, namely Australia, Belgium, Bulgaria, Canada, Czechoslovakia, Federal Republic of Germany, France, German Democratic Republic, Hong Kong, Ireland, Israel, Italy, Japan, Mexico, Netherlands, Poland, South Africa, Switzerland, Union of Soviet Socialist Republics, United Kingdom, United States of America, and Venezuela.

The Conference was organized and sponsored by the Science Council of Japan under the auspices of IOCG, and was cosponsored by IUCr, IUPAC, IUPAP, Japan Society of Applied Physics, and ten other Japanese academic societies. Financial support was provided by IUCr, IUPAP, Japanese industries, Japanese banks and other Japanese companies.

On the morning of 25 March, the Conference was officially opened by Prof. R. R. HASIGUTI, Chairman of the Organizing Committee of ICCG-4. The Opening Ceremony was followed by the Opening (plenary) Lecture, in which Prof. F. C. FRANK (UK) gave a fascinating lecture on 'Japanese Work on Snow Crystals'. Prof. FRANK reviewed and discussed the work on snow and ice crystals by the late Prof. U. NAKAYA and his pupils achieved in the first half of this century. It was interesting to note that there was an unusual snowfall during the Conference, which made Prof. FRANK's lecture even more impressive.

On the evening of 27 March Plenary lectures were given by Prof. S. AMELINCKX (Belgium) and by Dr. A. A. CHERNOV (USSR). Prof. AMELINCKX reviewed the present state of 'Characterization of Defects in Crystals' achieved by means of electron microscopy combined with electron diffraction. Dr. CHERNOV discussed the present state of theory on 'Stability of Faceted Shapes' or of singular interfaces. On the afternoon of 29 March, the Closing (plenary) Lecture was given by Dr. R. A. LAUDISE (USA), who assayed future prospects for various kinds of crystals in his lecture entitled 'Future Needs and Opportunities in Crystal Growth—Crystal Growth toward the Year 2000'.

Sixteen invited talks were concerned with various uptodate topics and actively investigated fields (names of coauthors not given):

- R. KERN (France) 'Mechanism of Epitaxy'
- M. J. STOWELL (UK) 'Initial Stages of Thin Film Formation'
- E. KALDIS (Switzerland) 'On the Rate-determining Steps in High-temperature Vapour Growth'
- M. B. PANISH (USA) 'Liquid Epitaxy of III-V Heterojunctions—System Thermodynamics and Fine Tuning of the Lattice Parameters'
- J. CHIKAWA (Japan) 'Video Display Technique for X-ray Topographic Images and its Application for Study of Crystal Growth'
- R. UYEDA (Japan) 'Morphology of Fine Metal Crystallites'
- P. BENNEMA (Netherlands) 'Crystal Growth from Solution—Theory and Experiment'
- F. SEKERKA (USA) 'Morphological Stability of Disc Crystals'
- J. D. LIVINGSTON (USA) 'Unidirectional Solidification of Eutectic and Eutectoid Alloys'

- A. HIGASHI (Japan) 'Growth and Perfection of Ice Crystals'
 K. S. BAGDASAROV (USSR) 'Growth and Perfection of High Temperature Oxides'
 A. R. LANG (UK) 'Glimpses into Growth History of Natural Diamonds'
 N. WATABE (USA) 'Crystal Growth of Calcium Carbonate in Biological Systems'
 S. ASAKURA (Japan) 'Ordered Biological Structures and their Growth'
 K. A. JACKSON (USA) 'Present State of the Theory of Crystal Growth from the Melt'
 W. T. STACY (Netherlands) 'Dislocations, Facet Regions and Growth Striations in Garnet Substrates and Layers'

More than 300 contributed papers together with the above invited papers were presented in three parallel sessions from the afternoon of 25 March, to the afternoon of 29 March. The papers were divided into the following 21 categories:

1. Theory and experimental studies on molecular mechanism
2. Morphological aspects—theoretical and experimental
3. Perfection and physical properties of crystals related to the growth process
4. Vapour growth (transport, chemical vapour deposition)
5. Thin films—fundamental aspects
6. Epitaxy, including liquid phase epitaxy
7. Solution (nonmetallic, including gel) growth
8. Flux growth
9. Hydrothermal growth, growth at high temperature and/or high pressure
10. Melt growth
11. Eutectic growth, convection, segregation
12. Solid-state crystallization, phase transition
13. Growth of polymer and biological crystals
14. Growth history of natural minerals
15. Growth of optoelectronic crystals
16. New technique of crystal growth
17. Scientific and educational cine films
18. Snow and ice
19. Whiskers
20. Liquid encapsulated Czochralski growth
21. Garnets, growth and properties.

Problems discussed in the Conference included, of course, orthodox topics such as molecular mechanism of growth, morphology, perfection, vapour growth, solution growth, melt growth, epitaxy, thin films, and so on. As to the kinds of crystals, electronics crystals were most actively investigated. The Organizers made an ambitious effort to expand the field of crystal growth to include biological crystals. Although they were not very successful in obtaining many contributed papers on biological crystals, there were two invited papers from the biological field.

As a whole the Conference was a great success in that it showed a very high scientific standard, and moreover it afforded a splendid medium for establishing international understanding among crystal growth people from various countries. The proceedings have been published in *Journal of Crystal Growth* [Vol. 24/25 (1974)] and reprinted in book form by North-Holland Publishing Co.

At the end of the Conference it was decided that ICCG-5 should be held in USA during 1977.

R. R. HASIGUTI

CONFERENCE ON LABORATORY INSTRUCTION IN CHEMISTRY

Troy, New York, 10-12 June 1974

The need for continuing evaluation of programmes in laboratory instruction and for identification of emerging trends was the motivation for conducting this Conference at the Troy campus of the Rensselaer Polytechnic Institute under the sponsorship of IUPAC. The 200 participants represented a wide geographic distribution (34 states and 5 Canadian provinces) and a spectrum of educational institutions ranging from large state universities to small liberal arts and developing urban colleges.

The programme was organized into five single sessions; each was devoted to a specific aspect of laboratory instruction and consisted of a plenary lecture followed by short contributed papers. The five areas included were: Laboratory Organization; The Integrated Laboratory; Instructional Aids and Equipment; Computers in Laboratory Instruction; and the General Chemistry Laboratory. Abstracts of the plenary lectures and contributed papers have been published in the January 1975 issue of *Journal of Chemical Education* (Vol. 52, pp. 27-45).

Many examples were presented illustrating ways in which the integrated or unified laboratory, which served to break down traditional boundaries in chemistry, was being developed successfully at different types of institution for both major and nonmajor students and at all levels of instruction. More evaluation of these programmes and followup of students in advanced undergraduate and graduate work and in industry were needed, however, to determine if the increased time and financial commitments were justified. A major emphasis continued to be towards more reliance on the investigative approach and on involving the student in the experimental planning so as to develop more of a research attitude and a feeling of personal accomplishment, although considerable discussion centred around the values of structured programmes versus openended projects. A consensus might be that both approaches were really necessary to provide adequate instruction in the basic skills of experimental chemistry as well as to stimulate enthusiasm for the scientific process. It was strongly pointed out, however, that there could be quite a difference in motivation and in appropriate objectives between a group of minority students in an evening urban college and chemistry majors at a small private liberal arts college or a large state university. The importance and diversity of laboratory aids and equipment—including computer-assisted instruction and uses of computers in laboratory management, direct online data acquisition, and simulation—were well recognized, and some spectacular uses of visual aids and instructional techniques were demonstrated; the greatly increased costs of these methods were often cited, however, and there was no unanimity as to the extent to which modern experimental apparatus should be understood by the student or used simply as a 'black box'. Finally, it was clear throughout the Conference by the manners of presentation, if not specifically stated in so many words, that excellent, exciting teachers and teaching assistants could be the most effective transmitters and catalysts of scientific enthusiasm.

R. L. STRONG

V IUPAC INTERNATIONAL SYMPOSIUM ON PHOTOCHEMISTRY

Enschede, 21-27 July 1974

The Symposium was attended by more than 200 participants from 20 countries, Austria (1), Belgium (10), Canada (6), Denmark (1), France (33), Germany (56), Greece (2), India (1), Ireland (3), Israel (2), Italy (8), Japan (4), Netherlands (28), Poland (2), Spain (1), Sweden (1), Switzerland (19), UK (15), USA (29), and Yugoslavia (1).

A special feature was a full-day session devoted to industrial applications of photochemistry. This session featured Dr. M. PAPE of BASF as the keynote speaker. The session was held on the first day in order that participants could become familiar with the problems early and have time for discussion throughout the course of the Symposium. The session included lectures by Dr. G. A. DELZENNE (Gevaert-Agfa), Dr. G. D. SHORT (ICI), Dr. A. REISER (Kodak), Dr. A. M. BRAUN (CIBA-GEIGY), Dr. W. KOCH (Sandoz), Dr. W. HERBST (Sandoz), and Dr. J. C. LANET (Rhône-Progil).

The second day of the Symposium featured plenary lectures by Prof. H.-D. SCHARF on 'Photocycloaddition of Dichlorovinylene Carbonate to Benzene and Naphthalene', Prof. F. WILKINSON on 'Triplet State Quenching by Coordination Compounds', and Prof. M. WRIGHTON on 'Generation of Catalysts by Photolysis of Transition Metal Complexes'. A special session on theoretical aspects of photochemistry and spectroscopy was held on the third day. This session was saddened by the death of Prof. T. FÖRSTER and the death of Prof. L. J. OOSTERHOF just prior to the Symposium. Both of these men were for many years major contributors to photochemistry and valued participants at previous Symposia in this series. The plenary lectures at this session were given by Prof. J. MICHL, 'Model Calculations of Photochemical Reactivity', Prof. A. DEVAQUET, 'Avoided Crossings in Photochemistry', and Prof. H. FISCHER, 'Magnetic Resonance in Photochemistry: Principles and Applications'.

Plenary lectures on the fourth day of the Symposium dealt with light-induced nucleophilic substitution and photooxidation. The programme began with Prof. J. CORNELISSE's lecture on 'Photosubstitution Reactions of Aromatic Compounds'. Prof. C. S. FOOTE summarized his work on singlet oxygen and the related topics of mechanism and energy transfer processes in dioxetane decomposition.

The final day dealt with physical methods in the study of photochemical processes. Prof. W. R. WARE spoke about the application of fluorescence quenching and exciplex photophysics. Prof. J. SALTIEL explored the role of the triplet state in the photochemical *cis-trans* isomerization of stilbene. The Symposium closed on a high level with Prof. D. SCHUSTER's discussion of the chemical and physical processes responsible for energy wastage in ketone photochemistry.

The Symposium featured a large number of shorter contributed papers in addition to the plenary presentations which have been mentioned. The success of the meeting was greatly enhanced by the fine quality of the short contributions. An experiment with parallel sessions devoted to short contributions in various areas was conducted. These sessions provided each speaker with a small audience expert in the field of the presentation. This enabled the speaker to eliminate much introductory material and greatly raised the quantity and quality of discussion. It offered the audience a choice of topics. The sessions were very well attended. The plenary lectures are

scheduled for publication in the official journal of IUPAC *Pure and Applied Chemistry*, Vol. 41, No. 4 (1975).

O. L. CHAPMAN

II INTERNATIONAL SYMPOSIUM ON MYCOTOXINS IN FOOD

Puławy, 23-24 July 1974

The Symposium was a continuation of the first meeting on control of mycotoxins held at Kungälv in 1972 and was held under the sponsorship of IUPAC and the Committees on Veterinary Sciences and Human Ecology of the Polish Academy of Sciences. It was coordinated by the Food Section of IUPAC (Chairman: Dr. R. MARCUSE) and the Veterinary Research Institute at Puławy (Director: Prof. M. TRUSZCZYNSKI) with an Organizational Committee consisting of Prof. M. NIKONOROW (Warsaw) Chairman, Prof. T. JUSZKIEWICZ (Puławy) Vice-Chairman, Dr. K. KOJIMA (Tokyo), Dr. P. KROGH (Copenhagen), and Dr. R. MARCUSE (Göteborg).

Some 75 participants were present, of whom 21 were from Poland. One general report and 40 scientific communications were presented. The aim was an exchange of experiences in the field of technology and chemistry of mycotoxins and other carcinogenic materials occurring in natural fodder and food products which might constitute a threat to human and animal health. The programme included discussions on the occurrence of mycotoxins and their potential threat for men and animals, the occurrence of prophylactics and detoxicants, pharmacodynamic properties and analytical methods.

The Symposium was opened by Prof. TRUSZCZYNSKI. Greetings were conveyed by Prof. A. RUTKOWSKI, Corresponding Member of the Polish Academy of Sciences and by Dr. R. MARCUSE, Chairman of the Food Section of IUPAC. A general report on the subject of the meeting was presented by Dr. A. D. CAMPBELL (Food and Drug Administration, Washington DC). Particular attention was paid to the potential threat of mycotoxins for human and animal health.

The scientific communications related to questions connected with the occurrence of various mycotoxins, including aflatoxins, ochratoxins, sterigmatocystine and zearalenone in feeds or feeding stuffs, in milk and meat and products based as these, and in vegetable products. The metabolism of aflatoxin and its effect on the immunology of some animals and pathogenic mechanism and recent achievements concerning biological and biochemical characteristics of the various mycotoxins were also discussed. Progress in studies on possible means of detoxicating contaminated feeds, a matter of considerable economic importance, was reviewed together with the mycotoxin control systems adopted by various countries. Detailed discussion on recent analytical methods, their scope and the difficulties encountered were also considered.

The mycotoxin problem was of great economic and health importance and was the subject of scientific research in many laboratories all over the world. There had been a rapid increase of publications with the consequent importance of confrontation of scientific opinions and facts in the form of direct contacts between the scientists concerned. The number of recognized mycotoxins and their metabolites significant for men and animals appeared to be steadily increasing. These could result in various pathological changes, such as the development of cancers, teratogenic changes, as well as considerable

economic losses in the modern animal production. The analytical aspects were associated with many methodical difficulties. Modern instrumental methods were necessary, including chromatography and in some cases mass spectrography or spectrofluorimetry.

There were, as yet, no effective and inexpensive methods for the destruction of mycotoxins in feeds and food products. This was a most important and urgent problem and prophylactic activity, control of consumption of the contaminated products being of particular importance. The Symposium presented a good opportunity for exchange of views and experience among specialists dealing with this problem, which was in the centre of interest of the modern toxicology. It brought together representatives of many active research centres from the whole world and gave an overall picture of the research work carried out during the last 2 years. The interchange of information constituted a valuable basis for future work.

On 23 July, a friendly meeting of the Symposium participants took place in the ruins of the Janowiec castle on Vistula. During this meeting the Polish national ensemble 'Powiśle' gave a performance, thus making the participants acquainted with the local folklore.

On 25 July, following the Symposium, participants took part in a study tour of the Refrigerator Storerooms in Lublin, where they saw storage methods of food products and the work of the laboratory. Participants also visited the former concentration camp Majdahek, the health resort of Nałeczów, and the ancient market-place at the town of Kazimierz on Vistula.

A. RUTKOWSKI

II AHARON KATZIR-KATCHALSKY CONFERENCE

Amsterdam, 2-6 September 1974

The Royal Netherlands Academy of Arts and Sciences acted as host for the Conference and cosponsored it in conjunction with IUPAC, IUPAP, European Molecular Biology Organization, Israel Academy of Sciences and Humanities, and the Aharon Katzir-Katchalsky Center of the Weizmann Institute of Science. All meetings were held in the main hall of the Trippenhuis in Amsterdam, with participants lodged in nearby hotels.

The Conference was opened on the morning of 2 September with the Chairman, Prof. M. MANDEL, welcoming the participants, in particular Dr. R. KATZIR, wife of the late AHARON KATZIR-KATCHALSKY, who took an active part in the meeting. A telegram from his brother Prof. E. KATZIR (President of Israel and a well-known molecular biologist himself) and a message from the President of the Israel Academy of Sciences and Humanities were read to the audience. Opening addresses were presented by Prof. H. B. G. CASIMIR (President of the Royal Netherlands Academy of Arts and Sciences) and by Prof. A. SILBERBERG on behalf of the Aharon Katzir-Katchalsky Center and IUPAC.

The Conference itself was organized essentially as a workshop with ample time for discussion. The general topic was 'Biopolymer Interactions'. The aim was to survey the field of interactions between biopolymers involved in the assembly of biologically active entities and to discuss the physical chemical aspects of these phenomena.

There were four consecutive sessions, each devoted to one of the following subjects:

1. chromatin

2. enzymes
3. viruses
4. ribosomes

Each subject was introduced by the presentation of two lectures: the first speaker expressed his view as a biochemist, the second as a physical chemist. Thereafter, a lively two-hour discussion took place. Each session ended the following morning with the presentation of a summary in which the speaker presented his personal views on the subject and the content of the discussions of the previous day. The names of the speakers and of those who presented the summaries in the four sessions were, respectively:

1. B. J. MCCARTHY (San Francisco)
G. FELSENFELD (Bethesda)
J. A. SUBIRANA (Barcelona)
2. L. A. AE. SLUYTERMAN (Eindhoven)
H. EISENBERG (Rehovot)
H. K. SCHACHMAN (Berkeley)
3. M. K. SHOWE (Haverford)
A. KLUG (Cambridge, UK)
E. KELLENBERGER (Basel)
4. M. NOMURA (Madison)
C. R. CANTOR (New York)
H. A. SCHERAGA (Ithaca)

In the course of the meeting an additional lecture by Dr. A. KLUG was intercalated to give him the opportunity of presenting to the audience his recent results on the structure of t-RNA. The workshop ended on the morning of 6 September with a panel discussion of all those who presented a summary on the prospects of research in their field.

Sixty scientists from different countries participated actively in the Conference. Most of them were experienced physical chemists or biochemists of established reputation: a few postgraduates and students were permitted to attend the meeting as well. It may safely be stated that all lectures not only were of high scientific standing, but were also presented in a particularly attractive and stimulating fashion. This was reflected in a high attendance at all lectures: few of the participants missed any of the sessions. In retrospect, it seems regrettable that the decision was made not to publish the proceedings of this workshop. The discussions were informal, but nonetheless far from superficial. In general they continued over lunch which all participants enjoyed together at the restaurant of the Doelen Hotel.

During the afternoon of 2 September, the Board of the Royal Netherlands Academy of Arts and Sciences received the participants with cocktails. On the night of 5 September the participants were the guests of the State Secretary of Education and Sciences, his excellency Dr. G. KLEIN and the Burgomaster and Elderman of the City of Amsterdam, in the Van Gogh Museum.

During the Conference special precautions were taken with respect to the safety of the participants. The most important measure taken probably was the complete lack of publicity (except in the scientific community). On advice of the Amsterdam Police a cruise through the canals at night was cancelled. Instead a visit to the Municipal Museum was organized at the last minute.

M. MANDEL

V INTERNATIONAL CONFERENCE ON ORGANIC PHOSPHORUS CHEMISTRY

Gdańsk, 16-21 September 1974

Organic phosphorus chemistry was one of the few branches of organic chemistry that had enjoyed particularly rapid development in the postwar years. This was due to the important role phosphorus compounds played in biological processes as well as to the wide practical applicability of some organic phosphorus compounds. Of great significance also was the fact that modern organic synthesis was closely connected with the development of organic phosphorus chemistry, and reactions such as those of WITTIG or HORNER-WITTIG had won a permanent place in chemical research with prospects for their application not yet fully explored. Furthermore, the fact that a phosphorus atom might occur in compounds with different valency, from two to six, accounted for the rapid development of studies on new structures, their spatial geometry, and reaction mechanisms. For these reasons symposia on organic phosphorus compounds usually attracted large numbers of participants from all over the world, representing both universities as well as industrial institutes and laboratories. This was also the case with the V International Conference on Organic Phosphorus Chemistry held on the campus of the University of Gdańsk.

The Conference was organized under the auspices of IUPAC and the Polish Chemical Society and was attended by 281 chemists from 18 countries. The largest groups of participants were from Poland (88), USSR, France, and Federal Republic of Germany (about 40 representatives each). The non-European countries represented included Australia, Canada, Japan, and USA.

After the welcoming address by Prof. J. MICHALSKI (Chairman of the Organizing Committee), the Conference was officially opened by Academician B. A. ARBUZOV (Honorary Chairman of the Conference). The participants were also addressed by Prof. WŁ. TRZEBIATOWSKI (President of Polish Academy of Sciences) and Prof. A. KJAER (President of the Organic Chemistry Division of IUPAC) who wished the participants fruitful discussions.

In the course of the Conference 17 plenary lectures and 74 short communications were presented. As during previous meetings in this series the plenary lecturers, selected by an International Scientific Committee, were of international reputation and authorities in their respective fields of phosphorus chemistry.

Both the plenary lectures as well as the short communications dealt with the most typical problems of phosphorus chemistry, recent developments in synthesis and reaction mechanisms, but the proceedings were dominated by stereochemical problems, especially the dynamic stereochemistry of pentacovalent phosphorus compounds. These were precisely the problems taken up by Prof. S. TRIPPETT (UK) in his inaugural lecture. He discussed in detail studies on determining apicophilicity of substitutes in trigonal bipyramidal pentacovalent phosphoranes and the effect of ringstrain on the stereochemistry of substitutions at phosphorus.

The papers of Prof. R. F. HUDSON (UK) and G. AKSNES (Norway) dealt with the formation of pentacovalent phosphorus compounds and their role and participation in organic reactions. Prof. R. BURGADA (France) reported on his results of studies on spirophosphoranes, with particular attention paid to the possibility of tautomeric equilibrium of the type $P^{III} \rightleftharpoons P^V$ in the case of spirophosphoranes with a P-H bond. Similar problems were discussed by

Prof. F. MATHIS (France), who reviewed in detail the physical and chemical properties of the P-N bond in a variety of types of organic phosphorus structure.

Prof. F. RAMIREZ (USA) presented a neat report on work done on elaboration of new methods of phosphorylation based on the oxyphosphorane concept, and Prof. C. B. REESE (UK) discussed nucleotide synthesis by the phosphotriester method. A very interesting lecture by Prof. J. G. VERKADE (USA) concerned configuration and conformation of monocyclic and bicyclic phosphorus esters, while Prof. J. MICHALSKI (Poland) discussed, among other matters, the application of cyclic phosphorus compounds to studies of the mechanisms of rearrangement of the type $P/O/SCN \rightarrow P/O/NCS$. Prof. W. G. BENTRUDE (USA) presented the state of knowledge on phosphoranyl radicals and discussed in detail their reactivity and configuration.

Academician A. N. PUDOVIK (USSR) discussed the latest achievements in the field of reactions of trivalent phosphorus compounds with carbonyl compounds and the paper of Prof. I. F. LUTSENKO (USSR) dealt with the problems of synthesis and reactions of dialkoxyposphines and new organometallic compounds. Prof. T. A. MASTRYUKOVA (USSR) discussed in detail the dual reactivity of phosphorus monothioacids with aliphatic diazo-compounds on the basis of extensive kinetic studies of this reaction.

Prof. K. ISSLEIB (German Democratic Republic) presented the very exhaustive work done by his research group on the synthesis of heterocyclic phosphorus compounds containing oxygen, sulfur, and nitrogen atoms in a molecule. Synthesis and properties of aromatic phosphorus heterocycles constituted an area developed in recent years by Prof. M. MÄRKL (Federal Republic of Germany), who presented his studies to the audience in a highly interesting way. Prof. J. H. BESTMANN (Federal Republic of Germany) dwelt on the application of organophosphorus compounds in the synthesis of cumulated ylides, and Prof. T. MUKAIYAMA (Japan) gave a comprehensive review of his extensive studies concerning the application of organophosphorus compounds in the synthesis of nucleotides and peptides. Application of molecular photoelectron spectroscopy to stereochemical problems in phosphorus chemistry was discussed by Prof. A. H. COWLEY (USA).

The professional standard of both the lectures and discussions was very high, which was recognized and appreciated by all participants. A number of organizational changes were made during the Conference. A meeting of the International Scientific Committee elected a coordinating body headed by Prof. J. MICHALSKI, which will decide on the organizers and the place of the next Conference. Also discussed was the problem of organizing joint conferences for organic and inorganic chemists working on phosphorus chemistry. It was decided that the plenary papers would be published in a special issue of *Phosphorus*. In addition to the main business of the Conference, a number of events were offered to the participants, such as sightseeing tours of Gdańsk and its vicinity, a cocktail party in Gdańsk Old Town Hall, and an excursion to Wdzydze Lake and picnic.

M. MIKOŁAJCZYK

II INTERNATIONAL SYMPOSIUM ON CHEMISTRY OF NONBENZENOID AROMATIC COMPOUNDS

Lindau, 23-27 September 1974

The Symposium was organized by Gesellschaft Deutscher Chemiker (GDCh) and sponsored by IUPAC. More than 180 chemists from numerous European countries as well as from Canada, Cuba, Israel, and USA participated in the meeting; in particular there was present an important group of Japanese university professors and scientists as well as German students.

The meeting was opened by the President of GDCh, Prof. H. HANSEN, who cordially welcomed the participants from 12 countries. As a specific object in view of GDCh, Prof. HANSEN mentioned the active advancement of actual chemical developments; in this connexion he emphasized the special merits of Prof. E. HÜCKEL, Honorary President of the Symposium. Because of his fundamental ideas about the electronic structure of aromatic compounds, scientific progress on this field was definitely influenced. Prof. K. HAFNER, Chairman of the Symposium, gave a summary of the present level of the chemistry of nonbenzenoid aromatic compounds.

As official representative of IUPAC, Prof. H. ZOLLINGER (Vice-President of the Organic Chemistry Division) took part in the meeting; the official deputy of the Chemical Society of Japan was Prof. T. NOZOE, who took the initiative for the excellently organized first meeting in this series (ISNA I: Sendai, 1970).

According to the specific standard of ISNA I, internationally recognized scientists reported in 11 plenary lectures about more recent important developments in the field of nonbenzenoid aromatic compounds. In more than 30 contributed lectures chemists from universities and industry reported about experimental and theoretical advances made since ISNA I. Main effort had been concentrated on syntheses and reactions of cyclic conjugated polyenes and new heterocycles. Special attention was paid to modern spectroscopic methods for the solution of structure and bonding problems as well as the quantum chemistry of π -systems.

The plenary lectures of the Symposium were to be published in *Pure and Applied Chemistry* [scheduled Vol. 44, No. 4 (1975)], the official journal of IUPAC, and as a specially bound reprint. The abstracts of the contributed papers were published by GDCh in a booklet for the participants at the meeting.

Amongst the plenary lecturers, Prof. A. G. ANASTASSIOU (USA) reported about the 'Synthesis and Study of Select Heterocycles'. Particular emphasis was placed on the recognition of key steric and electronic factors controlling the development of heteroaromaticity as well as heterohomoaromaticity and heterobicycloaromaticity. The review was devoted to the hetero[9]annulenes, their benzologues, and the hetero[13]annulenes, respectively, and incorporated information attesting to the validity of HÜCKEL's $4n+2$ rule. The existence of bicycloconjugation in the 9-heterobicyclo[4, 2, 1]nona-2, 4, 7-triene system was documented by experimental results and the 2-heterobicyclo[3, 2, 1]octa-3, 6-diene skeleton was presented as a system with the ability to realize a homoconjugated frame.

Prof. V. BOEKELHEIDE (USA) presented an interesting account about 'Intrusion of Substituents into the Cavity of Aromatic π -Electron Clouds'. The bridged [14]annulenes were exceptional models for testing theories and providing quantitative data. For the dihydropyrene system it was demon-

strated that diatropic ring current effects on chemical shifts were of the same magnitude for carbon-13 as for hydrogen for the same position in space relative to the aromatic π -electron cloud. The continuing need for additional samples of bridged [14]annulenes had led to the development of new synthetic methods. On this basis it was possible to realize the syntheses of bridges [18]annulenes, tetra-bridges cyclophanes, and substituted [2.2]metapara-cyclophanes. The latter substances provided opportunity for quantitative measurement of the interaction of substituents with aromatic π -electron clouds.

Prof. M. J. S. DEWAR (USA) gave a comprehensive and stimulating review about 'Studies of some Nonbenzenoid Aromatic Systems'. A new version (MINDO/3) of the MINDO semiempirical SCF MO method had been developed. MINDO/3 seemed to avoid the serious defects of earlier treatments and gave results at least comparable with those of the best *ab initio* SCF procedures at one-hundred-thousandth of the cost. Calculations were reported for the benzyne, and for various cyclic polymethines, including $(\text{CH})_3^+$, $(\text{CH})_3$, $(\text{CH})_3^-$, $(\text{CH})_4$, $(\text{CH})_5^+$, $(\text{CH})_5$, $(\text{CH})_5^-$, $(\text{CH})_9^+$. Theoretical information was given for azulene and pentalene, for the cycloheptatriene-norcaradiene equilibrium, and for spiroononetetraene. The advanced approach led to new results for silabenzene, for a variety of polyazines and polyazoles, and for various aromatic and potentially aromatic sulfur-containing compounds.

Dr. P. J. GARRATT (UK) discussed recent developments in the area of 'Polycyclic Systems Containing Small-membered Rings'. The syntheses of a number of polycyclic systems containing potential cyclobutadiene rings were summarized. The main route to these compounds involved a bis-Wittig reaction with a compound containing a 4-membered ring. The spectroscopic properties of the compounds were correlated with the structure. In those cases in which delocalization occurred, the nuclear magnetic resonance spectra were consistent with these systems having a paratropic contribution from the 4-membered ring. In the case of 2-thianorbiphenylene, the paratropic component could be removed by oxidation to 2-thianorbiphenylene 2, 2-dioxide. The electronic spectra of biphenylene, 2-thianorbiphenylene, and tetraphenyl-2, 5-dithiabisnorbiphenylene were found to be similar.

Prof. H. GÜNTHER (Federal Republic of Germany) informed about 'Results of ^{13}C -nmr Spectroscopy in the Field of Cyclic Conjugated π -Electron Systems'. The theoretical basis for the interpretation of carbon-13 chemical shifts was reviewed briefly and ring current contributions to the shielding of the ^{13}C -nucleus were discussed in detail. The recent advances were illustrated by examples from the field of polycyclic nonbenzenoid π -systems and bridged annulenes. The fingerprint nature of ^{13}C -nmr data was stressed and the significance of σ -bond structure demonstrated for bridged [14]-annulenes and related compounds. Pyrene and the two isopyrenes dicyclopenta[ef,kl]haptalene and dicyclohepta[cd,gh]pentalene served as model compounds to illustrate typical features of ^{13}C -nmr spectra of alternating and nonalternating π -systems. The sensitivity of ^{13}C -nmr for the detection of valence isomerizations was exemplified with results obtained for 11,11-disubstituted 1.6-methano-[10]-annulenes.

Prof. E. HEILBRONNER (Switzerland) presented a critical synopsis on 'Photoelectron Spectra of Nonbenzenoid Cyclic Conjugated π -Electron Systems'. In an introduction the theoretical principles and practical limitations were outlined. On this basis the photoelectron spectra of three types of nonbenzenoid system were discussed: crossconjugated, nonalternant π -

Systems (6-vinyl-fulvene, heptafulvene, and sesquifulvalene); benzologuetropones [4, 5-benzotropone, 4, 5-(2', 3'-naphtho)-tropones and a series of alkyl substituted derivatives]; bridges [14]annulenes and dicyclohepta[cd,gh]-pentalene. The photoelectron spectroscopic data of this π -system and the results known to date for benzenoid hydrocarbons, linear polyenes, azulenes, bridged [10]annulenes, did not allow the formulation of yet another 'aromaticity' criterion.

Prof. Y. KITAHARA (Japan) summarized the experimental results about '8-Oxoheptafulvene'. The research in this field was initiated by chemical and physical studies of heptafulvene. 8-Oxoheptafulvene, which had both heptafulvene and ketene moieties, displayed several modes of cycloaddition reaction with various olefins and ketones. Depending on the reactants, the initial cycloadducts underwent further rearrangement reactions or extrusion of carbon dioxide. Particularly the reactions with tropones provided an elegant one step synthesis of heptafulvalenes.

Prof. S. MASAMUNE (Canada) pointed out some experimental and theoretical aspects of 'Degree of Electron Delocalization in Small-ring Systems'. For the synthesis of [4]annulene and the CH^+ -adduct an elegant approach was developed. The square pyramidal adduct of [4]annulene of C_{4v} symmetry was predicted by quantum chemistry and had been characterized by spectroscopic and chemical methods. The current state of theoretical development was illustrated by the treatment of [4]-annulene. The properties of methyl tri-*tert*-butyl[4]annulene-carboxylate—a derivative of [4]annulene, perturbed slightly by substituents—had been fully elucidated, including its X-ray crystallographic analysis. The experimental results led to the conclusion that a rectangle, distorted slightly by substituents, corresponded to the most stable conformation of this [4]annulene system. It was almost certain that the ground state of the parent [4]annulene was singlet and the geometric structure was rectangular with two short bonds of approximately 1.37 Å and two longer ones of the order of 1.51 Å.

Prof. M. NAKAGAWA (Japan) reported on the exhaustive work on 'Acetylene-Cumulene'-Dehydroannulenes'. For the synthesis of tetrasubstituted tetrahydro[18]- and [22]-annulenes containing a diacetylene and a hexapentaene unit, a general approach was elaborated, which consisted of the reductive dehydroxylation of corresponding 18-membered and 22-membered cyclic glycols. On this basis an important method for preparation of tetrasubstituted didehydro[4n+2]annulenes containing an acetylene and a butatriene unit had been developed. The didehydro[4n+2]annulenes ($n = 3 \sim 7$) were diatropic compounds with high conformational stability. A synthetic route for the preparation of didehydro[14]annulenes annelated with naphthalene or benzene was described, and the effect of annelation on π -electron delocalization of the annulene ring discussed.

Prof. G. SCHRÖDER (Federal Republic of Germany) gave a systematic survey of 'Higher Membered Annulenyl Ions'. The annulenyl ions were evaluated by three questions:

- bond delocalization or scope of validity of HÜCKEL's rule,
- chemical properties,
- configurational and/or conformational stabilities.

Especially stereochemical questions were discussed, starting with carbo- and heterocyclic-annulenes, then turning to the aza[13]- and the aza[17]-annulenylanion and the [17]-annulenyl anion.

R. KREHER

II INTERNATIONAL CONGRESS ON INDUSTRIAL WASTE WATER AND WASTES

Stockholm, 4-7 February 1975

Under the sponsorship of IUPAC and cosponsorship of the International Association on Water Pollution Research (IAWPR), the Federation of Swedish Industries arranged this International Congress on Industrial Waste Water and Waste problems. It was organized by the staff of the Swedish Water and Air Pollution Research Laboratory. The Congress, which attracted more than 700 participants from about 30 nations, was a follow up of the earlier International Congress on Industrial Waste Water which took place in Stockholm during November 1970. The initiative for the second Congress was taken by the Section on Water Quality of IUPAC which also constituted the Programme Committee.

Plenary sessions were held on the first and last days. On the second and third days the programme was divided into sections, each covering an industrial branch where the problems from an environment protection point of view were similar. In this way was included those types of industries which had the most severe problems with waste water and wastes. The following industries were covered:

- Metal and metal processing industries
- Chemical industries
- Pulp and paper industries
- Food industries

In the final sessions the subjects of 'Monitoring to Control Effluents' and 'Relation of Treatment and Ecological Effects' were treated. As main speakers some 17 experts had been invited and in addition about 70 discussion papers were presented by Congress participants.

The Congress was opened by His Majesty the King of Sweden and the introductory lecture was given by Dr. H. RODERICK, head of the environment directorate of OECD Paris. Dr. RODERICK claimed that, in order to restore the damage of environment on a greater scale, effective cooperation over boundaries was necessary. Within OECD some progress had been made concerning measures against industrial pollution and dumping of chemicals over boundaries. But much more was to be done before the situation could be described as good. The fears that costs for environment protection measures would lead to unwanted competitive situations for industries in different countries, had not been proved to be true.

From the proceedings in the industrial sessions the following could be mentioned. The organization of waste banks had proved to be a promising way to handle chemical wastes especially, claimed Dr. H. O. BOUVENG. Waste banks had now been organized in Federal Republic of Germany, Netherlands, and Scandinavia. Cooperation between the responsible organizations in the different countries had resulted in that waste quantities had been subject to import and export.

Different techniques to treat waste water from the pharmaceutical industry were demonstrated in a couple of papers. Biological treatment in plastic packing filters and stepwise distillation were among those techniques which were described more thoroughly. The use of activated carbon for treatment purposes was presented in a number of papers. A. NETZER reported a laboratory investigation of the removal of colour in waste water from textile

factories by treatment with activated carbon and polymeric resin adsorbents. Most interesting were the new polymeric resins which were built up the same as common ion-exchange resins. These resins were more easy to adopt to special treatment purposes than activated carbon and often had a longer lifetime. Unfortunately, a simple and cheap method of regeneration, which was a condition for more widespread use of the relatively expensive resins, were not yet available.

J. HØK presented work in which activated carbon and reverse osmosis were compared for the treatment of textile waste water. G. WALTER spoke about some practical experiences from treatment of industrial waste waters with activated carbon, while S. E. JØRGENSEN reported on an investigation which had been carried out with activated carbon for treatment of waste water containing phenol. P. BJÖRKLUND presented a liquid-liquid extraction process for the recovery of acid and metals from stainless steel pickle baths. A full scale plant was in operation at a Swedish Steel Mill.

G. R. WEBSTER demonstrated a closed system for eliminating magnesia from aluminium scrap and A. DUNEWALL described a system for recovery of oil from used cutting fluids with recovery of the treatment chemical, aluminium sulfate. A promising technique for destruction of cyanidic hardening salts was described by G. SAMUELSON. In this process the salt was treated with steam under pressure and high temperature in order to hydrolyze the cyanides to formates and ammonia.

J. WENZEL gave a survey of the recovery of waste fibre. He demonstrated that, in spite of the fact that the total amount of recovered fibre had increased six times between 1964 and 1973, the ratio between production of recovered fibre and virgin fibre had not increased, but remained constant at about 20%. A comparative study of treatment of waste water with biological technology at 7 mills producing fibre building board in USA was presented by J. A. OLESZKIEWICZ.

S. SELANDER reported on his experiences from a fibre building board mill in France, which had a totally closed backwater-system. A. WONG presented a paper about colour removal of waste waters from pulp mills by treatment with high molecular weight amines. J. C. MULLER reported a method of treatment for pulp and paper waste water with respect to toxic substances by foam separation. A technique to produce compost earth from fibre sludge was described by T. YAMAGUSHI. K. FORSS presented the Pekola Protein Process in which the carbon hydrates in waste sulfite liquor was fermented to proteins.

In the session on 'Monitoring Control Effluents', a new Nordic project for the study of the total monitoring of processes and waste water streams from pulp and paper industries was presented. P. SOLYOM described a working system for toxic substances in waste waters going to municipal sewage treatment plants.

During the sessions on 'Relation of Treatment and Ecological Effects', K. WUHRMAN stated that freshwater systems were very sensitive for new and in nature nonoccurring chemicals, which were synthesized and produced with increasing frequency. Another urgent demand was that the discharge of phosphorus and hard degradable chemicals to inland waters must be decreased.

R. ROSENBERG claimed that the ecosystems in brackish waters were not more sensitive than those in a marine environment, as had been claimed previously. L. CARTER demonstrated that fishing was a more severe threat than the discharge of effluents into the North Sea.

The main lecture papers presented at the Congress would be published in

the IUPAC journal *Pure and Applied Chemistry* during 1976, while the discussion papers were to be published by IAWPR.

B. GÖRANSSON

INTERNATIONAL SYMPOSIUM ON MACROMOLECULES

Jerusalem, 13-18 July 1975

The 24th International Symposium on Macromolecules also constituted the III Aharon Katzir-Katchalsky Conference. Some of the distinguished visitors recalled that in April 1956, some 19 years earlier, they had participated in an International Symposium on Macromolecules in Rehovot and Jerusalem organized by the late AHARON KATZIR-KATCHALSKY, to whom the present Symposium was dedicated.

The Symposium was under the auspices of IUPAC, Israel National Academy of Sciences and Humanities, Israel Chemical Society, and Aharon Katzir-Katchalsky Center at the Weizmann Institute of Science. Prof. H. BENOÎT, President of its Macromolecular Division, officially represented IUPAC; Prof. G. SMETS, Secretary of the Division, represented the Royal Belgian Academy of Arts and Sciences; and Prof. A. SILBERBERG was Chairman of the Organizing Committee. Participation included about 200 scientists from 21 different countries and about 100 Israeli registrants. The size of the Conference enabled proceedings to be held in the beautiful and effective adjoining facilities graciously offered by the Israel Academy and the Jerusalem Van Leer Foundation. Three convenient lecture rooms, within close proximity of each other, a cafeteria, meeting and reception rooms, created a pleasantly relaxed and efficient atmosphere. Most hotels being conveniently situated nearby enabled participants to take advantage of the beautiful Jerusalem summer climate by walking to and from the various sessions and social functions. Organizational facilities, both inside and outside the lecture rooms, functioned smoothly and efficiently. International symposia had in recent years grown to almost unmanageable sizes. The not excessive attendance at the present meeting led to a relaxed, intimate atmosphere extremely conducive to scientific discussions and social interchange.

The scientific aspects of the Symposium were rewarding. A central feature was the four plenary lectures which attracted most of the participants. J. TH. G. OVERBEEK discussed 'Polyelectrolytes, Past, Present and Future'; D. S. BRESLOW—'Biologically Active Synthetic Polymers'; F. R. EIRICH—'Polymers and other Composites'; and E. KATZIR (President of the State of Israel) discussed 'Macromolecules as Immobilized Catalysts and as Control Elements in Chemical Reactions'. A special Symposium on Frontiers of Macromolecular Science was held in honour of Prof. HERMAN MARK on his 80th birthday and, in a series of seven short papers, physical structural and synthetic aspects of polymerization processes were discussed intensively. In a slightly different vein, J. PRAWER of the Hebrew University spoke on 'Heavenly and Earthly Jerusalem between Judaism and Christianity', at the opening ceremony on the Hebrew University Campus. In an impressive function at the residence of the President of Israel, Prof. KATZIR presented Prof. MARK with a certificate commemorating the planting of 80 trees on the occasion of his birthday.

The main flow of lectures proceeded in three parallel sessions. Lectures were organized in nine separate sections which were keynoted by sectional lectures. In the section on Surface and Electrochemistry, J. LYKLEMA discussed 'In-

ference of Polymer Adsorption from Double Layer Measurements'; in Physicochemical Aspects, W. PECHHOLD spoke on 'Present Theories of the Condensed Polymer State' and R. J. RUBIN on 'Characterization of the Shape of Polymer Chains'; A. YAMAKAWA could not attend for reasons of health but his paper on 'Statistical Mechanics of Wormlike Chains' would be included in the volume of the IUPAC journal *Pure and Applied Chemistry* containing the plenary and sectional lectures. A particularly active section was devoted to the topical subject of Ions and Polar Groups in Polymeric Solids; R. E. BARKER lectured on 'Mobility and Conductivity of Ions into and in Polymeric Solids', and A. EISENBERG on 'Structure and Viscoelastic Properties of Ion-containing Polymers in the Solid State'.

In Polymer Reactions, another very active field, H. KAGAN spoke about 'Graphite Insertion Compounds as Chemical Reagents in Organic Chemistry', and A. PATCHORNIK on the 'Use of Polymeric Reagents in Organic Synthesis'. In the section on Synthetic Membranes, O. KEDEM discussed 'Selectivity of Polyelectrolyte Membranes', and A. S. MICHAELS dealt with 'Synthetic Polymeric Membranes, Practical Applications—Past, Present and Future'. It was by now apparent that, along with the more theoretical and academic aspects, topical practical implications, of major relevance of the world today, were stressed to a very high degree. In the field of Pollution Abatement R. KUNIN discussed the 'Use of Macroreticular Polymeric Adsorbents for Treatment of Waste Effluents' and H. STRATHMAN 'Membrane Separation Processes in Advanced Waste Water Treatment'. Under Biomedical Applications, S. D. BRUCK described 'Polymeric Materials in the Physiological Environment, in Composites and Special Systems', R. N. HAWARD reported on the 'Provision of Toughness in One- and Two-phase Plastics', and J. C. HALPIN on 'Structure-Property Concepts for Polymeric Systems'. Finally, in the section on Fibres, we heard G. TESORO on 'Current Research in Chemical Modifications of Cellulosic Fibres', and J. H. BRADBURY on the 'Morphology and Chemical Structure of Wool'.

It was unfortunate that lack of space does not allow mention in this short report of the many short contributions which blended well into the general framework outlined above. As there was not a single topic it would be impossible to bring in here a critical discussion centering around a single problem. On the contrary this meeting had, once more, shown that Polymer Science was a vital and creative science and furthermore that it contributed to human welfare on a very broad front. It was mentioned that Polymer Science had, in the past year, reached two milestones of major importance: the award of the Nobel Prize to PAUL FLORY and our very young Geheimrat MARK reaching the age of eighty. We are looking forward to further progress and exciting discoveries and of course to the next Macromolecular Symposium. Good luck to our Japanese colleagues for 1977.

H. EISENBERG

FORTHCOMING IUPAC-SPONSORED SYMPOSIA

II IUPAC SYMPOSIUM ON PHOTOCHEMICAL PROCESSES IN POLYMER CHEMISTRY

Leuven, 2-4 June 1976

The Symposium is being held on the Katholieke Universiteit Leuven campus in Heverlee under the auspices of IUPAC and sponsored by the Ministry of Education and the National Fonds voor Wetenschappelijk Onderzoek.

Scientific Programme

A series of plenary lectures covering the different aspects of photochemistry as related to the polymeric field, the topics of which are mentioned below, are scheduled. Contributions related to each of these topics are invited, and will be discussed in a session following the related plenary lecture. Extended abstracts (5 pages) of these communications are to be submitted in three copies to the Secretary; 15 March 1976 is the deadline for receipt of abstracts. In order to ensure easy copying, the text should be typewritten on DIN A4 first quality paper, **double** spaced, leaving a 2-cm margin on all sides.

The invited lectures, which will be published in the official journal of IUPAC *Pure and Applied Chemistry*, are as follows:

Prof. N. TURRO (USA) 'Energy Transfer Processes'

Dr. H. WINSLOW (USA) 'Photooxidation of High Polymers'

Prof. A. LEDWITH (UK) 'Photoinitiation of Polymerization, including Charge Transfer Complexes'

Dr. J. WILLIAMS (USA) 'New developments in Photoimaging Processes'

Prof. G. GEUSKENS (Belgium) 'New Aspects of Energy Transfer Phenomena in High Polymer Systems including Degradation Phenomena'

Prof. G. WEGNER (Federal Republic of Germany) 'Solid State Polymerization Mechanisms (including Comparison with the Hasegawa Four Center Polymerization)'

Dr. J. PEARSON (USA) 'Photoconductivity of High Polymers'

Prof. M. KRYSZEWSKI (Poland) 'New Developments in Photochromic Polymers and Related Phenomena'

Dr. A. TROZZOLO (USA) 'Photochemical Reactions in High Polymers'

Prof. J. FAURE (France) 'Laser Spectroscopic Methods for Study of Primary Processes during Photodegradation'

Lodging, Meals, Transportation

To ensure maximum exchange and ease of operation, lodging should be arranged through the Symposium Secretariat. All participants will be lodged in Leuven and vicinity. Transportation between lodging facilities and the meeting site will be arranged. The prices for the rooms (bed and breakfast) are single room 850 BF, double room 1,000 BF. To enhance exchange of ideas participants are encouraged to lunch together. Tickets will be on sale at the information desk.

Secretariat

All enquiries concerning the meeting should be addressed to:

Prof. F. C. DE SCHRYVER
Secretary IUPAC Microsymposium 1976
Department Scheikunde
Katholieke Universiteit Leuven
Celestijnenlaan 200 F
B-3030 Heverlee, Belgium

The registration fees are 2,000 BF, students 1,000 BF, accompanying persons 800 BF.

V INTERNATIONAL CONFERENCE ON NONAQUEOUS SOLUTIONS

Leeds, 6-9 July 1976

The Conference and accommodation will be at Bodington Hall, a University of Leeds Hall of Residence in pleasant surroundings on the northern perimeter of the city. Most of the accommodation will be in single rooms.

Main Topics

- A. Preparations and reactions in nonaqueous media
- B. Solvation and solution processes:
 - B1. Physicochemical aspects, thermodynamics, kinetics, mechanisms, ion-association, *etc.*
 - B2. Spectroscopic methods of solvation and structure determination
- C. Molten salts
- D. Liquid metals and metals in liquids

The following plenary lectures, which will be published in *Pure and Applied Chemistry*, have already been arranged:

- J. L. DYE (USA) 'Cation-Electron Interactions in Metal Solutions—from Solvated Electrons to Alkali Anions'
- M. C. R. SYMONS (UK) 'Application of ESR Spectroscopy to Study of Solvation in Nonaqueous Solvents'
- J. F. COETZEE (USA) 'Influence of Solvent Properties on Ligand Substitution Mechanisms of Labile Complexes'
- F. SEEL (Federal Republic of Germany) 'Coloured Sulfur Species in EPD-Solvents'
- J. VEDEL (France) 'Analytical Studies of Chemical Reactions in Molten Salts'

In addition to the plenary lectures there will be seven halfday sessions in which time will be available for about 80 contributed papers (20 minutes each). There will also be six invited session lectures (40 minutes each; also to be published in PAC) aimed at reviewing special topics. The deadline for submission of abstracts is 31 January 1976.

The official language of the Conference will be English. No translation facilities will be available. Speakers who wish to present a paper in another language will be asked to distribute a written text in English.

Secretariat

All correspondence should be sent to the Secretary of the Organizing Committee:

Dr. J. B. GILL
Department of Inorganic and
Structural Chemistry
University of Leeds
Leeds LS2 9JT, UK

1976 PRAGUE MEETINGS ON MACROMOLECULES Prague, 12-16 July 1976

The two meetings detailed below will be held simultaneously at the Technical University in Prague. The scientific programmes will be so arranged that there will be no clash in the main lectures presented at both meetings.

V Discussion Conference: Phases and Interfaces in Macromolecular Systems

1. *Phase behaviour, concerning amorphous and mesomorphic phases.* Thermodynamic and kinetic interpretation of the coexistence, composition, and morphology of the separated phases and microphases. Mutual compatibility of polymers. Polymeric mesomorphic phases (liquid crystals).
2. *Interface phenomena:* Structure and properties of interfaces, including conformation of macromolecules at the interface. Surface and interface tension. Adsorption of macromolecules and its effect on the stability of dispersions.

Theoretical and experimental aspects of the formation and coexistence of amorphous and mesomorphic phases and of the general properties of the phase boundaries in polymer systems will be discussed, as well as the influence of the interface phenomena on the phase behaviour. *Crystalline phases and polymer fractionation will not be included.*

XVI Microsymposium: Advances in Scattering Methods

1. *Neutron, X-ray, and light small angle scattering*
2. *Classical light scattering by small and larger particles*
3. *Spectroscopy of thermal and stimulated light scattering*

Contributions dealing with advanced neutron, X-ray, and light scattering methods will be appreciated. Assuming that each method consists of three components (*viz.* theory, technique, and instrument), at least one of them should be new, nonconventional or, in any case, must represent an important contribution to or substantial improvement of a 'classical' method. *Applications of known methods to a new subject should be avoided* (except when this application might substantially extend the scope of the method).

Secretariat

Further information and registration forms are available from:

PMM Secretariat
c/o Institute of Macromolecular Chemistry
Czechoslovak Academy of Sciences
CS-162 06 Prague 616-Petřiny
Czechoslovakia

VIII INTERNATIONAL SYMPOSIUM ON CARBOHYDRATE CHEMISTRY

Kyoto, 16-20 August 1976

The Symposium is being organized by the Science Council of Japan under the sponsorship of IUPAC. The scientific programme will include plenary lectures by several invited speakers, and the presentation of general papers which may cover the following topics:

1. Organic and physical chemistry of carbohydrates
(synthesis, reaction mechanism, conformation, stereochemistry, *etc.*)
2. Polysaccharides
(animal, plant, and microbial polysaccharides; structure, conformation, biosynthesis, chemical synthesis, metabolic enzymes, *etc.*)
3. Complex carbohydrates
(glycolipid, glycoprotein, cell surface carbohydrate, and other biologically active carbohydrates; structure, function, metabolism, immunochemistry, *etc.*)
4. Advances in analysis of carbohydrates
(chemical, enzymatic, and instrumental analyses, *etc.*)
5. Industrial and medical aspects of carbohydrates
(chemically and biologically active derivatives and new types of polysaccharide for industrial and medical uses, *etc.*)

English will be the official language at the Symposium. Abstracts of papers should be written also in English. The plenary lectures will be published in the official journal of IUPAC, *Pure and Applied Chemistry*.

General Information

Group flights from Europe and North America may be available if the number of participants travelling together from certain places either in Europe or North America is satisfactory to form a tour group. Japan Air Lines (JAL) will be appointed as the official carrier. Full details will be available shortly together with information on hotel accommodation.

A social programme for active and associate members during the Symposium is planned for the enjoyment of their stay in Kyoto. Kyoto, an ancient capital of Japan for more than ten centuries, is the cradle of Japanese culture and is an undoubted gem of never-failing attraction to visitors from any part of the world.

Correspondence

All correspondence relating to the Symposium should be addressed to:

Dr. A. MISAKI, General Secretary
VIII International Symposium on Carbohydrate Chemistry
c/o Kyoto International Conference Hall
Takara-ike, Sakyo-ku
Kyoto 606, Japan

INTERNATIONAL SYMPOSIUM ON ANALYTICAL CHEMISTRY IN THE EXPLORATION, MINING, AND PROCESSING OF MATERIALS

Johannesburg, 23-27 August 1976

The Symposium is being held under the auspices of IUPAC and organized by the Council for Scientific and Industrial Research in association with a number of South African organizations. It will take place on the campus of the Rand Afrikaans University and aims to highlight the role of analytical chemistry in the exploration for raw materials, their beneficiation, refining, and in the production of materials. The Symposium will be of particular interest to analytical chemists, physical chemists, metallurgists, chemical and mining engineers, geochemists and geologists, managers and those persons interested in the quality of materials.

Scientific Programme

Plenary lectures on the analytical needs in the production and use of such materials as coal, ferrous and nonferrous metals, precious metals, *etc.*, will be delivered. Further plenary lectures, devoted to various analytical techniques, will also be presented.

Plenary Speakers will be, *inter alia*:

Prof. V. A. FASSEL (USA)

Dr. D. FRITZ (USA)

Prof. J. GIJBELS (Belgium)

Dr. R. HÄGSTROM (USA)

Dr. W. HOOK (UK)

Prof. H. IRVING (UK)

Mr. R. JENKINS (USA)

Dr. G. KÖLLING (Federal Republic of Germany)

Dr. K. LAQUA (Federal Republic of Germany)

Mr. R. MICHAELIS (USA)

Dr. K. OHLS (Federal Republic of Germany)

Mr. S. SMALLBONE (USA)

Prof. J. C. VAN LOON (Canada)

Dr. A. WALSH (Australia)

Dr. J. WEBB (UK)

Parallel sessions (research papers) will be held covering all facets of the Symposium, viz:

Prospecting and mining

Metals

Coal

Instrumental analytical techniques

Classical and modern chemical techniques

Standard reference materials

Automation

Computation

To enable delegates to learn of the problems confronting analytical chemists in the many facets of modern technology, analytical methods used at present and associated problems will be discussed during special discussion sessions.

Copies of extended abstracts of all papers will be available to delegates at

Registration. All plenary lectures will be published in the official IUPAC journal *Pure and Applied Chemistry*. It is not intended to publish *in extenso* the contributed papers, but extended reports of the Symposium may be published in selected scientific journals. The official language of the Symposium will be English. Limited facilities for translation may be available.

An exhibition of scientific instruments and equipment of particular interest to delegates will be arranged.

General Information

Block reservations at suitably located, medium-priced hotels are being made by the organizers. South African Airways have been appointed as official carriers for the Symposium. In addition to social functions there will be some technical tours and other visits arranged for delegates. An interesting ladies' programme of local tours is possible if there is sufficient interest. Various sightseeing post-Symposium tours are available on request.

Enquiries and Information

Please address communications to:

Conference Division (IUPAC Symposium)
Council for Scientific and Industrial Research
POB 395, Pretoria 0001
Republic of South Africa

VII INTERNATIONAL MASS SPECTROMETRY CONFERENCE

Florence, 30 August-3 September 1976

This Conference is being organized by the Commission of the European Communities and by the Italian Chemical Society on behalf of an international scientific committee, comprising representatives from Australia, Belgium, Czechoslovakia, Denmark, France, Germany, Italy, Japan, Netherlands, Norway, Sweden, Switzerland, UK, USA, USSR, and Yugoslavia. It will be held in the 'Palazzo dei Congressi' in Florence under the sponsorship of IUPAC.

The scientific programme will be planned around the following topics:

Theory in mass spectrometry (including QET, MO, basic aspects of ionization, energy distribution and transfer), metastable ion studies, reaction analysis (including kinetics, thermodynamics, ion-molecule reactions), instrumental developments and data processing, ionization techniques, organic analysis (including fragmentation mechanisms and related isotopic analysis), inorganic analysis (including cluster ions), isotopic analysis (including nuclear materials, geochronology, space), environmental (including GC/MS, mass fragmentography), biochemical and medical.

Leading world authorities in these fields will be invited to present review papers. Contributed papers on these and related topics will also be included. Poster session are also foreseen (see, e.g., *Science* **184**, No. 4144, p. 1361). Each scientist can have space on which to post his graphs, photos, and data. Therefore, simultaneously with others, he has approximately 1.5 hours in which to discuss his work with anyone who is interested.

Abstracts of contributed papers should be submitted by 5 January 1976 for consideration by the International Scientific Committee and they will be scrutinized by two referees. The abstract should be 300-500 words long. It should include an introductory statement indicating concisely the purpose of the work and a closing statement summarizing the significant new results. The decision on paper acceptance will be based on the abstracts. A few selected references to closely related information should be listed at the end of the abstract. These references are only for the information of the Referring Committee and should not be quoted in the text of the abstract. Authors who intend to participate in poster sessions only should also submit an abstract of 300-500 words by 5 January 1976.

General Information

Florence is a very popular tourist centre and accommodation will be limited and difficult to obtain in hotels. Therefore accommodation has been arranged by, and should be booked through, the Organizing Committee. Accommodation at preferential rates has been reserved in the modern 'Student House', where delegates for the whole week will be allocated preferentially. Block bookings have also been made in Florence hotels.

A Conference Dinner and other social activities, as well as a programme for the ladies, are being arranged. Charter flights and package holidays before and after the Conference are under consideration. The registration fee, which will include a book of extended abstracts, will be about \$90. The charges for the conference dinner and any planned excursions will be extra.

Secretariat

For more detailed information on the technical programme, social activities, accommodation costs, and package holidays, please contact:

Dr. S. FACCHETTI
Joint Research Centre EURATOM
I-21020 Ispra (VA)
Italy

MICROSYMPOSIUM ON LONGTERM PROPERTIES OF POLYMERS AND POLYMERIC MATERIALS

Stockholm, 30 August-1 September 1976

The Symposium will be held under the auspices of IUPAC at the Royal Institute of Technology. It will treat the material as a chemical subject where the polymer properties are related to:

- (a) Thermal and Mechanochemical Reactions
- (b) Chemical and Photochemical Reactions
- (c) Biological Reactions
- (d) Reuse and Disposal Problems

These four subtitles are also the subdivisions of the Symposium. Papers related to pure rheological and other mechanical subjects will be referred to the VII International Rheology Congress (see p. 160) for consideration.

The scientific programme will consist of invited lectures and contributed

papers. The following scientists have been invited to give symposium and main lectures:

HERMAN MARK (USA)
GERALD SCOTT (UK)
N. GRASSIE (UK)
S. N. ZHURKOV (USSR)
K. L. DEVRIES (USA)
H. H. G. JELLINEK (USA)
E. KÜSTER (FRG)
D. M. WILES (Canada)
T. V. KAGIYA (Japan)
J. E. GUILLET (Canada)

Participants intending to contribute papers are asked to provide the title and a summary (300 words) by 1 December 1975. The selection of the contributed papers will be made by the Scientific Programme Committee. An accepted paper will be given 15 minutes for presentation. The invited lectures and the contributed papers will be published as one or two symposium volumes. Instructions about manuscripts will be given when the contributions are accepted.

The use of English as the Symposium language is recommended. Only papers in English can be published.

General Information

A registration fee of 300 Sw. Kronor will be charged to the participants. This fee will include participation in the scientific sessions and the social programme, and also includes a copy of the summaries of the invited lectures and the contributions. A special programme will be arranged for accompanying participants of the Symposium (registration fee 100 Sw. Kronor).

Scandinavian Airlines System (SAS) has been appointed the official carrier for participants travelling by air. Rooms for the participants will be reserved in hotels and student dormitories within walking distance or a short subway ride from the Symposium.

Correspondence

All correspondence and inquiries concerning the symposium should be addressed to:

Prof. BENGT RÅNBY
Department of Polymer Technology
Royal Institute of Technology
S-100 44 Stockholm 70, Sweden

III IUPAC CONFERENCE ON PHYSICAL ORGANIC CHEMISTRY

Montpellier, 6-10 September 1976

The Conference is sponsored by IUPAC in conjunction with Société Chimique de France and Société de Chimie Physique. The central theme will deal with the study of the $>C=X$ bond ($X=O, S, N$): theoretical aspects, structure, and reactivity. The following topics will be considered:

(a) Theoretical calculations and physical properties of the $>C=X$ bond

- (b) Nucleophilic addition reactions and their retroversion if any
Addition of Grignard reagents, metal hydrides, and other nucleophiles
Hydrolysis of imines, ketals, thioketals, orthoesters, including glycosides and other natural products
- (c) Enolization reactions, ketonization of enols, and hydrolysis of vinyl ethers
- (d) Hydrolysis of esters, nitriles, amides, and peptides

Emphasis will be given to the stereochemical course of these reactions, and to any catalytic process involved:

acid-base and nucleophilic, intramolecular and/or bifunctional, micellar and enzymatic catalysis.

The following persons have already accepted to give a plenary lecture:

F. G. BORDWELL (USA)

C. A. BUNTON (USA)

B. CAPON (UK)

J. E. DUBOIS (France)

W. P. JENCKS (USA)

W. KUTZELNIGG (Federal Republic of Germany)

A. RASSAT (France)

F. H. WESTHEIMER (USA)

The plenary lectures will be published in *Pure and Applied Chemistry*, official journal of IUPAC. The programme will allow for the presentation of a limited number of contributed papers on topics directly related to that of the Conference.

English and French will be the official languages of the Conference; arrangements for simultaneous translation will not be made. Papers, abstracts, and oral presentations should preferentially be in one of these two languages.

Correspondence

All correspondence concerning the Conference should be addressed to:

Prof. G. LAMATY

Laboratoire de Chimie Organique Physique

Université des Sciences et Techniques

du Languedoc

Place Eugène Bataillon

F-34060 Montpellier Cedex

France

XVII INTERNATIONAL CONFERENCE ON COORDINATION CHEMISTRY

Hamburg, 6-10 September 1976

The Conference is being organized by Gesellschaft Deutscher Chemiker under the sponsorship of IUPAC. It will be held at the University of Hamburg. The majority of the scientific sessions will take place in the University Chemical Institute.

Scope

The Conference will be concerned with recent developments of coordination chemistry in the following fields:

1. Structure and bonding
2. Novel synthetic routes
3. Kinetics and reaction mechanisms
4. Catalytic and technological aspects
5. New types and concepts in coordination compounds
6. Bio-coordination chemistry

Plenary Lectures

The following distinguished scientists have accepted invitations to deliver plenary lectures during the Conference:

J. CHATT (UK)	'Prospect and Retrospect: 25 Years ICCC'
H. HARTMANN (FRG)	'25 Jahre Ligandenfeldtheorie'
J.-M. LEHN (France)	'Cryptates: Macropolycyclic Cation Inclusion Complexes'
P. L. PAUSON (UK)	'Aromatic Transition-Metal Complexes: The First 25 Years'
H. SCHÄFER (FRG)	'Koordinationsverbindungen in der Gasphase'

Section Main Lectures

F. CALDERAZZO (Italy)	'Synthetic and Mechanistic Aspects of Insertion Reactions'
N. CALDERON (USA)	'Synthetic and Mechanistic Aspects of Olefin Metathesis'
J. FALBE (FRG)	'Koordinationsverbindungen als Katalysatoren in großtechnischen Prozessen'
J. HALPERN (USA)	'Mechanisms of the Substitution and Oxidative Addition Reactions of Platinum (O) and Related Complexes'
R. H. HOLM (USA)	'Biological Aspects of Coordination Chemistry'
F. JELLINEK (Netherlands)	'Structural Aspects of Organotitanium Chemistry'
S. OLIVE and G. HENRICI-OLIVE (Switzerland)	'Coordination and Catalysis'
C. SCHÄFFER (Denmark)	'Parametric Analysis of Ligand Field Spectra Using the Non- additive and the Additive Model Field'
A. SHILOV (USSR)	'Multielectronic Processes in Coordination-Catalysis'
P. L. TIMMS (UK)	'Direct Synthesis with Metal Atoms'
M. E. VOL'PIN (USSR)	'Recent Development of N ₂ -Fixation by Transition Metal Compounds'

It is likely that an additional section main lecture may be presented.

Abstracts of the scientific contributions will be printed and distributed at the congress office. Plenary lectures will be published in the IUPAC journal *Pure and Applied Chemistry*. The official languages of the Conference will be English, French, and German.

General Information

Hamburg offers excellent and extensive hotel accommodation in every price range. Hotel reservations will be handled by 'Fremdenverkehrszentrale Hamburg'. Inclusive tours from several airports to Hamburg will be offered by Deutsches Reisebüro GmbH (DER), Kongressverbindungsstelle Hamburg, D-2000 Hamburg 36, Hohe Bleichen 13, for participants from abroad outside the responsibility of the organizers. The Organizing Committee wishes to offer possibilities to renew old contacts and to establish new ones. A variety of social events will therefore be offered and a special Ladies Programme will be arranged.

Correspondence

All correspondence concerning the Conference should be sent to

Dr. W. FRITSCHÉ
Secretariat of XVII ICCC
c/o Gesellschaft Deutscher Chemiker
POB 900440
D-6000 Frankfurt/Main 90
Federal Republic of Germany

XVIII INTERNATIONAL CONFERENCE ON COORDINATION CHEMISTRY

São Paulo, 18-23 July 1977

The Conference is being organized by the Brazilian Academy of Sciences, under the sponsorship of IUPAC, and will take place at the University of São Paulo.

Papers will be presented and discussed under five main headings:

1. Organometallic Compounds
2. Mechanisms of Reactions of Complexes
3. Structure and Stereochemistry of Coordination Compounds
4. Applications of Coordination Compounds in Analytical Chemistry
5. Lanthanide Chemistry

The following persons will deliver plenary lectures, which will be published subsequently in the IUPAC journal *Pure and Applied Chemistry*:

E. O. FISCHER (Federal Republic of Germany)
H. TAUBE (USA)
S. KIRSCHNER (USA)
H. M. N. H. IRVING (UK)
E. GIESBRECHT (Brazil)

The official language of the Conference will be English, though papers may be presented in any other language. Speakers in other languages are recommended to distribute a written text in English at the presentation of their contribution.

Correspondence

All correspondence relating to the Conference should be addressed to:

Prof. PASCHOAL SENISE
Instituto de Química
Universidade de São Paulo
Caixa Postal 20780
São Paulo, Brazil

26th IUPAC CONGRESS

Tokyo, 4-10 September 1977

The Congress will be held in the Akasaka area of Tokyo under the auspices of the Science Council of Japan. It is also supported by the Chemical Society of Japan, Pharmaceutical Society of Japan, and the Agricultural Chemical Society of Japan. The tentative scientific programme will consist of Joint Symposia and Division Sessions.

The Joint Symposia have been particularly organized with the recognition that the future of mankind, its prosperity and even its survival, should be largely dependent on the progress of fundamental and applied chemistry, and that interdisciplinary cooperation amongst various specialists is urgently needed. Subsessions Ia-Ie have been so chosen as to represent those fields which could provide useful approaches for solving the entrusted problems.

Sessions II-V correspond to the IUPAC Divisions: Physical, Analytical, Organic, and Macromolecular Chemistry, respectively.

- I. Joint Symposia on Chemistry for the Welfare of Mankind
 - Ia. Selectivity and Specificity in Chemical Reactions
 - 1. *Selective and Specific Reactions*
 - 2. *Selectivity and Specificity in Preparative Chemistry*
 - 3. *Interpretation of Selectivity and Specificity*
 - Ib. Phase Boundaries and Multiphase Systems
 - 1. *Liquid-liquid Interphases, Micelles, and Liquid Crystals*
 - 2. *Membranes*
 - 3. *Reactions on Solid-phase Boundaries*
 - Ic. Biologically Active Substances
 - 1. *Structure-Activity Relationships*
 - 2. *Metabolism and Biosynthesis*
 - 3. *Mode of Action*
 - 4. *Effects on the Environment*
 - Id. Separation and Detection of Trace Species
 - 1. *Environmental Systems*
 - 2. *Biological Materials*
 - 3. *Industrial Materials*
 - 4. *Migration and Circulation of Chemical Species through Atmosphere, Hydrosphere, and Lithosphere.*
 - Ie. Modern Aspects of Industrial Materials and Resources
 - 1. *New Industrial Materials including Medical Materials*
 - 2. *Contribution of Chemistry to Food and Food Stock Problems*
 - 3. *New Sources of Energy and Materials*

- II. Physical Chemistry Section
 - 1. *Application of Lasers*
 - 2. *Structures and Dynamics of Excited Species*
 - 3. *Novel Methods for Structure Determination*
 - 4. *Systems with Unusual Valences*
 - 5. *Molecular Dynamics—Nonequilibrium States and Chemical Relaxation*
- III. Analytical Chemistry Section
 - 1. *Methodology for Characterization of Materials*
 - 2. *System Chemical Analysis*
 - 3. *Complex-formation in Analytical Chemistry*
 - 4. *New Instrumental Methods in Analytical Chemistry*
- IV. Organic Chemistry Section
 - 1. *Structure-Reactivity Relationships*
 - 2. *Syntheses Leading to Compounds of Special Interest*
 - 3. *New Information through Mathematical and Physical Methods including Computer Calculations*
 - 4. *Chemistry of Natural Products*
- V. Macromolecular Chemistry Section
 - 1. *Macromolecular Design and Characterization*
 - 2. *Excited States of Polymer Systems*
 - 3. *Rheology and Relaxation Processes*
 - 4. *Synthetic Macromolecules of Biological Interest*
 - 5. *Structure, Superstructure, and Properties of Polymers*

Language

The official language of the Congress is English. Although presentation of the contributed papers may be made in any language, the Organizing Committee hopes that the language will be understandable to most of the attendants to facilitate active discussion of the paper. No simultaneous translation service will be provided.

Invited Lecturers

Distinguished scientists from various countries of the world are expected to deliver plenary, opening, and session lectures at the Congress. The following persons have already accepted an invitation:

- H. BENOÎT (France)
- M. CALVIN (USA)
- A. ESCHENMOSER (Switzerland)
- P. D. LAFLEUR (USA)
- E. O. FISCHER (FRG)
- Y. KITANO (Japan)
- G. PORTER (UK)
- C. D. RITCHIE (USA)
- S. SOURIRAJAN (Canada)

Contributed Papers

Those who wish to present a contributed paper in the Congress are requested to return the provisional application form not later than 31 August 1976. The final application and the abstract of the paper should be submitted not later than 15 March 1977. The author will be notified concerning acceptance of the paper at a later date.

Accommodation and Travel

The Organizing Committee has appointed Japan Travel Bureau Inc. (Convention and Tour's Section, Head Office) as the official travel agent. Details of group flights from North America and Europe will be announced in due course.

Correspondence

All correspondence concerning the Congress should be addressed to:

26th IUPAC Congress
POB 56, Kanda Post Office
Tokyo 101-91, Japan

IV INTERNATIONAL CONGRESS OF PESTICIDE CHEMISTRY

Zürich, 24-28 July 1978

The scientific programme will consist of symposia, workshops, and discussion sessions. To avoid an excessive number of parallel section-meetings it is planned to devote an average of 2 days to each main topic. Plenary lectures and a major portion of the papers presented will be given by invited speakers. Contributed papers and short communications, which any participant may submit, will be screened by the Scientific Programme Committee and, depending on their scientific quality and novelty, be referred to symposia, workshops, or discussion sessions.

The programme has been planned to include the following main topics:

Plenary Session

World Food Production, Environment, Pesticides

Sections

- I Synthesis of Pesticides (including industrial aspects)
- II Chemical Structure and Biological Activity (including toxicological activity)
- III Natural Products with Biological (pesticidal and growth-regulating) Activity
- IV Biochemistry of Pests and Mode of Action of Pesticides (including resistance mechanisms)
- V Degradation (including chemical structure and degradability)
- VI Pesticide Residues (including instrumentation and methods)
- VII Formulation Chemistry
- VIII Education in Pesticide Chemistry (tentative)

The official language of the Congress will be English. No simultaneous translation will be provided.

Secretariat

Enquiries and correspondence concerning the Congress should be addressed as follows:

IV International Congress of Pesticide Chemistry
POB 182
CH-4013 Basle
Switzerland

ASSOCIATED ORGANIZATIONS OF IUPAC

VII INTERNATIONAL CONGRESS ON RHEOLOGY

Gothenburg, 23-27 August 1976

The Congress will be held at Chalmers University of Technology under the auspices of the International Committee on Rheology. The Swedish Society of Rheology, a section of the Swedish National Committee for Mechanics, will act as the host organization.

All aspects of rheology are within the scope of the Congress. Contributions that aim at a reduction of the diversity of the theoretical and empirical framework by introducing new unifying concepts will be especially welcome. Increasing evidence pointing towards far reaching similarities in the flow behaviour of substances with widely varying structure seems to support such an approach.

Scientific Programme

The scientific programme will consist of invited and contributed papers. The contributed papers will be published as brief scripts, containing the main results, illustrations, and tables. These scripts will in no way preclude subsequent full publication. Together with the full text of the invited lectures, the scripts will constitute the Proceedings of the Congress.

The use of English as the Congress language is recommended. No simultaneous translation will be provided.

General Information

A registration fee of 500 Skr will be charged to participants in the Congress. This fee will include participation in the scientific sessions and social functions. It also includes a copy of the Congress Proceedings. The Congress banquet is not included. Reduced fees will be charged to students and to persons accompanying Congress participants.

Rooms for the participants have been reserved in hotels and student halls of residence within walking distance of the Congress. A social programme and a special ladies programme will be arranged. During the Congress, there will be an exhibition of rheological measuring devices and related equipment.

Correspondence

All correspondence and inquiries concerning the Congress should be addressed to:

Prof. JOSEF KUBÁT
Chalmers University of Technology
Fack
S-402 20 Gothenburg 5
Sweden

INTERNATIONAL COUNCIL OF SCIENTIFIC UNIONS

INTERNATIONAL SYMPOSIUM ON ARID LANDS IRRIGATION IN DEVELOPING COUNTRIES

ENVIRONMENTAL PROBLEMS AND EFFECTS

Alexandria, 16-21 February 1976

The Symposium has been convened by COWAR and organized jointly by COWAR, UNESCO, the Academy of Sciences and the Ministry of Irrigation of Egypt, in cooperation with FAO, WHO, IASH, IAH, ICID, ICOLD, ISS, IUBS, and IUPAC, and with the support of UNEP. All technical sessions will be held in the Hotel San Stefano.

Origin and Purpose

This Symposium was initiated and is being planned by COWAR as a multi-disciplinary study within the context of international activities orientated towards arid lands irrigation. It will follow the UN World Food Conference (Rome, November 1974), the ICID Congress on Irrigation and Drainage (Moscow, August 1975) and the 2nd World Congress on Water Resources (New Delhi, December 1975). It is expected that the meeting will have an important input, not otherwise provided, to the UN Water Conference (Buenos Aires, second half of March, 1977).

It will survey world experience in research and its application in arid land irrigation, with emphasis on water use and on the environmental effects of irrigation. It will be followed by a Regional meeting of MAB Project 4: Impact of human activities, on the dynamics of arid and semi-arid zones ecosystems, with particular attention to the effects of irrigation (24-28 February 1976) and a SCOPE/COWAR/MAB/UNEP working group will assess its results during the period 16-28 February.

Scientific Programme

The papers in English and/or French to be presented at the Symposium, all of which have been invited, will be preprinted and will be distributed free of charge to the participants. Opening speeches, general reports, summaries of discussions and conclusions will be printed after the Symposium.

Eight plenary Sessions (mornings and afternoons of 4 working days) will be concerned with the topics and will include the invited speakers. The programme for each Session has been arranged in consultation with the appropriate governmental and nongovernmental international organizations. Each Session will be coordinated by a general reporter.

Session 1—Areas and methods

The purpose will be to set the scene and to indicate the interest of the organizations particularly concerned.

Session 2—Case studies

In order to emphasize the need to bring all appropriate scientific disciplines to bear on each irrigation project, a number of case studies will be presented for discussion.

Session 3—Influence of irrigation on hydrological processes: quantity and quality

The most profound changes are expected in the soil moisture zone and the water-table aquifers. Evapotranspiration, and thus the atmospheric part of the hydrological cycle, may be modified by irrigation. The maintenance of higher moisture content in the soil, resulting from irrigation, may lead to increases in surface runoff from precipitation because of decreased infiltration.

Session 4—Land use, soils, and water quality

Emphasis will be placed on problems of secondary salinization, alkalinization, and water-logging related to irrigation and drainage. Methods of predicting and preventing these harmful processes, as well as numerical methods for forecasting, modelling and controlling them, will be included. The balance of water and salts in soils, closely related to the subjects of Session 3, and the influence of irrigation on the natural environment, will be discussed.

Session 5—Effects of irrigation on the biological balances of the environment

Ecological changes brought about by irrigation projects in arid areas are among the greatest of human influences on the natural environment. The species and distribution of plants and animals are almost totally changed and this affects the terrestrial, aquatic, and atmospheric environments. This Session is designed to analyse some of these changes, laying emphasis on those which are amenable to environmental management.

Session 6—Efficiency of irrigation schemes

Low returns from irrigation investments are often due to ineffective use of irrigation methods. These lead to reduced interest of the farmers and, as a result, the management and maintenance of the system suffer. The basic requirements of effective irrigation will be presented, including the technical aspects of irrigation efficiency as such, as well as the operational management and socioeconomic aspects.

Session 7—Human problems in irrigation areas

It is expected that the discussions will include assessment of sanitary and public health problems, the effects of water-borne diseases and the way to control them, environmental health and sanitation, organization of basic health services and health education, experience in resettlement in irrigated areas, and psychosocial aspects of resettlement.

Session 8—Synthesis: Reports of working groups and conclusions

During the Symposium, working groups will examine certain questions in more detail than in the general Sessions and will draft conclusions. Working groups will report back at this final Session.

Correspondence

All correspondence about the Symposium should be addressed to:

Mr. GAMUL ABDEL SAMIE
Vice-President, Academy of Sciences
Organizing Committee for COWAR Symposium
102 Kasr el Aini Street
Cairo, Arab Republic of Egypt

ICSU ABSTRACTING BOARD

ICSU AB has recently announced the availability* of the following publications:

Primary Publications and Secondary Services, Partners in Information Flow

This publication contains the papers presented at a Conference arranged by ICSU AB in cooperation with the Royal Society, where problems of mutual concern to primary editors and secondary services were discussed. The purpose of the Conference was to give editors of primary publications, especially of scientific and technological journals, an insight into the problems of abstracting and indexing services, and to provide an opportunity for discussion of problems of mutual interest.

178 pages

\$18.00 plus mailing charges

Proceedings of General Assembly Meeting (Berlin, July 1974)

The first part of this publication refers to the plan for developing cooperation between Abstracting and Indexing Services: Methodology for an Aggregate List and Methodology for coverage allocation. Position statements on UNISIST and Developing Countries are given in the second part. The third part deals with activities of ICSU AB Members in all aspects of scientific and technical information. The fourth part reports a discussion on the 'Role of Abstracting and Indexing Services in Storage of Data'. The fifth part comprises reports concerning copyright problems. Examples of cooperation are given in the sixth part. Part seven refers to reports on benefits of common practices for Abstracting and Indexing Services and Users.

260 pages

\$20.00 plus mailing charges

Guidelines for the Coded Bibliographic Strip for Serial Publications

The coded bibliographic strip is designed to provide accurate, unambiguous, and concise identification of serial publications and articles contained within issues of serial publications. Such precise identification is essential to efficient and effective transfer of information from producers of the serial literature to the users. In computer-based bibliographic control and information processing systems the use of accurate, highly compact identification codes becomes an economic necessity. The coded bibliographic strip printed by the producers of the serial literature, *i.e.*, the publishers on the covers of their primary and secondary publications, provides this identification. The adoption of the use of the coded bibliographic strip by primary and secondary serial publishers is encouraged by UNESCO, ICSU AB, and ISDS.

16 pages

\$5.00 plus mailing charges

International Classification for Physics (1975)

The publication of this first issue of the ICSU AB 1975 Classification Scheme for Physics marks a new step forward in cooperation between the world's Abstracting and Indexing Services. The new classification, representing broad international agreement between American, British, French, and German

*From ICSU AB Secretariat, 17 Rue Mirabeau, F-75016 Paris, France.

services, together with active participation of the world's physicists themselves, allows bridges to be built for the exchange of information between Abstracting and Indexing Services to help eliminate costly duplication of work. In its present form the classification covers the core areas of physics, and comprises 1,200 classes and subclasses. There are four hierarchical levels, each level being understood in the context of its broader class.

40 pages

\$10.00 plus mailing charges

ENVIRONMENTAL POLLUTANTS—SELECTED ANALYTICAL METHODS

The Scientific Committee on Problems of the Environment (SCOPE) was established by ICSU in 1969 (a) to advance knowledge of the influence of man and his activities on his environment, as well as the effects of these alterations on man, his health, and his welfare, with particular attention to those influences and effects which are either global or shared in common by several nations; and (b) to serve as a nongovernmental, interdisciplinary, and international council of scientists and as a nongovernmental source of advice for the benefit of governments and intergovernmental agencies with respect to environmental problems.

Much of the work of SCOPE is concerned with the effects of small or trace quantities of a variety of chemical elements and compounds in various segments of the environment, in air, water, soil, and biota. The determination of trace amounts of certain substances entails difficulties. It is obviously of paramount importance that results obtained in various parts of the world be strictly comparable, and the present volume—SCOPE 6—presents a number of carefully chosen analytical methods for use by those seeking advice on the choice of method.

SCOPE 6 was compiled by the Working Group on Methodology of Determination of Toxic Substances in the Environment, which was composed of experts from IUPAC: W. GALLAY (Canada)-Chairman, H. EGAN (UK), J. L. MONKMAN (Canada), R. TRUHAUT (France), P. W. WEST (USA), G. WIDMARK (Sweden).

Contents: Introduction. Determination of Airborne Particulate Lead by Atomic Absorption Spectrophotometry. Determination of Airborne Particulate Cadmium by Atomic Absorption Spectrophotometry. Determination of Airborne Particulate Zinc by Atomic Absorption Spectrophotometry. Determination of Airborne Particulate Copper by Atomic Absorption Spectrophotometry. Determination of Airborne Particulate Nickel by Atomic Absorption Spectrophotometry. Determination of Airborne Particulate Manganese by Atomic Absorption Spectrophotometry. Determination of Airborne Particulate Cobalt by Atomic Absorption Spectrophotometry. Determination of Airborne Particulate Beryllium by Atomic Absorption Spectrophotometry. Determination of Airborne Particulate Vanadium by Atomic Absorption Spectrophotometry. Determination of Chromium in Airborne Particulates by Atomic Absorption. Determination of Airborne Particulate Hexavalent Chromium. Determination of Airborne Particulate Lead by the Ring Oven Technique. Determination of Airborne Particulate Zinc by the Ring Oven Technique. Determination of Airborne Particulate Copper by the Ring Oven Technique. Determination of Airborne Particulate Nickel by the Ring Oven Technique. Determination of Airborne Particulate Cobalt by the Ring Oven Technique. Determination of Airborne Particulate Beryllium by the Ring Oven Technique. Determination of Selenium in Air. Determination of Particulate Arsenic in Air. Determination of Mercury in Air. Determination of Mercury in Water. Determination of Mercury in Biological Media. Determination of Methylmercury Compounds in Fish. Determination of Traces of Lead and Cadmium in Water. Determination of Total Lead and Cadmium in Biological Media. Determination of Selenium in Biological Media. Determination of Sulfur Dioxide by the West Gaeke Method. Collection and Determination of Sulfur Dioxide Incorporating Permeation and West Gaeke Procedure.

Determination of Atmospheric Sulfur Dioxide by Coulometric Titration. Method for the Continuous Determination of Carbon Monoxide in the Atmosphere by Nondispersive Infrared Spectrometry. Determination of Carbon Monoxide in the Atmosphere by Flame Ionization Detection. Estimation of Nitrogen Dioxide and Nitric Oxide in Air. Determination of Ozone in the Atmosphere. Spectrophotometric Determination of Atmospheric Fluorides. Spectrophotometric Determination of Nitrate in Air. Determination of Sulfuric Acid Aerosol by the Ring Oven Technique. Determination of Fluoride in Water. Spectrophotometric Determination of Nitrate in Water. Determination of Phosphate in Water—Method 1 (High Level). Determination of Phosphate in Water—Method 2 (Low Level). Determination of Dissolved Oxygen in Water. Estimation of DDT and Related Compounds Together with Polychlorobiphenyl Compounds in Biological Media. Estimation of Traces of Polychlorobiphenyl Compounds (PCB). Determination of Benzo(a)pyrene and Benzo(k)-fluoranthene in Airborne Particulates.

xiv+277 pages

Butterworths

£7.00

IUPAC COLLEAGUES DECEASED

We have been informed of the death of:

- Canada* Dr. N. F. BRIGHT (26 November 1974)—Commission on High Temperatures and Refractory Materials (1970-1973)
- Israel* Prof. E. D. BERGMANN (6 April 1975)—Bureau (1971-)
- UK* Dr. H. J. BUNKER (8 August 1975)—Section on Fermentation Industries (1963-1969)
- USA* Dr. B. RIEGEL (20 May 1975)—US Delegation to XXIV, XXV, and XXVI IUPAC Council Meetings (1967, 1969, and 1971)

FOUR IMPORTANT NEW PUBLICATIONS AVAILABLE FROM IUPAC SECRETARIAT

Analytical Methods for Use in Occupational Hygiene

A further supplement to *Analytical Methods for Use in Occupational Hygiene* has been published in the IUPAC journal *Pure and Applied Chemistry* Vol. 40, No. 3 (1974). It comprises eight methods prepared by the IUPAC Section on Air Quality: Determination of airborne particulate vanadium (by spectrophotometry), of lead, cadmium, and vanadium (by atomic absorption spectrophotometry), and of benzo[a]pyrene and benzo(k)fluoranthene (by chromatography and optical fluorescence); Performance standards for detector tubes; Particulate lead in air; Hydrogen chloride vapour in air.

The first material in this series was published in 1959 under the title *Methods for the Determination of Toxic Substances in Air* for inclusion in a looseleaf binder. First and Second Replacement-Additions were issued in 1962 and 1969, respectively. In 1969, the title was revised to *Analytical Methods for Use in Occupational Hygiene* to enlarge the scope. The original publication and the two Replacement-Additions (supplements), which did not appear in *Pure and Applied Chemistry*, are available from Butterworths, Borough Green, Sevenoaks, Kent TN15 8PH, UK.

The present supplement (Third Replacement-Addition) is available from the IUPAC Secretariat as a reprint (58 pages) from *Pure and Applied Chemistry* and is suitable, after punching, for insertion in a looseleaf binder or may be used as such. Price \$4.00 (£1.33) surface post or \$5.25 (£1.75) airmail.

Basic Definitions of Terms Relating to Polymers

Two broad sets of definitions presented in this document have been compiled by the IUPAC Commission on Macromolecular Nomenclature. One of these is based on the structure of polymer molecules and the other on the processes by which polymeric substances come into being. The first type of definition is termed 'structure-based' and the second 'process-based'. This document updates and supersedes the reports issued by IUPAC on the subject in 1952, 1962, 1965, 1966, and 1968, as well as Tentative Nomenclature Appendix No. 13 (February 1971) to the *IUPAC Information Bulletin*.

Published in *Pure and Applied Chemistry* Vol. 40, No. 3 (1974) and available as a reprint (16 pages) from the IUPAC Secretariat, price \$1.50 (£0.50) surface post or \$2.25 (£0.75) airmail.

Recommended Reference Materials for Realization of Physicochemical Properties

There are many measuring systems and instruments in use today which yield results whose uncertainty of measurement and limits of error cannot be established without the employment of materials with known properties. Materials used for this purpose are called reference materials. In 1972 the IUPAC Commission on Physicochemical Measurements and Standards published a 'Catalogue of Physicochemical Standard Substances' in *Pure and Applied Chemistry* (Vol. 29, No. 4, pp. 597-616).

However, it was realized that a more comprehensive compilation was needed and a Sub-Commission on Calibration and Test Materials was set up to prepare recommendations on the selection and specification of reference materials for use in various types of physicochemical measurement. The first

batch of the Sub-Commission's recommendations have now been issued in sections dealing with General Introduction (to the whole series), Enthalpy, Optical Rotation, and Surface Tension. Further sections will be published as more recommendations become available.

Published in *Pure and Applied Chemistry* Vol. 40, No. 3 (1974) and available as a reprint (82 pages) from IUPAC Secretariat, price \$6.00 (£2.00) surface post or \$8.00 (£2.66) airmail.

Nomenclature of Carotenoids

Although IUPAC issued 'Rules for Nomenclature of Carotenoids' as early as in 1947 and later in 1951, many subsequent developments in the carotenoid field have resulted in situations that are not now covered adequately. For example, the number of known naturally occurring carotenoids has increased from some 80 to about 300. Since 1965 the IUPAC Commission on Nomenclature of Organic Chemistry and the IUPAC-IUB Commission on Biochemical Nomenclature have been engaged in revising the Rules. The updated recommendations were first issued in 1972 as Tentative Nomenclature Appendix No. 19 to the IUPAC *Information Bulletin* and were widely circulated throughout the world for comment. The present Rules (approved 1974) have been published after the two Commissions had taken into consideration the comments so received.

The 13 Rules cover the following:

Class of compound; The stem name; Specific names—end group designations; Numbering of carotenoid hydrocarbons; Nor carotenoids and seco carotenoids; Changes in hydrogenation level; Oxygenated derivatives; Numbering of oxygenated derivatives; *retro* Nomenclature; Apo nomenclature; Higher carotenoids; Stereochemistry; Trivial names. An Appendix gives a listing of naturally occurring carotenoids having trivial names with their systematic names and structures.

Published in *Pure and Applied Chemistry* Vol. 41, No. 3 (1975) and available as a reprint (approx. 28 pages), price \$3.00 (£1.00) surface post or \$4.00 (£1.33) airmail from the IUPAC Secretariat.

IUPAC MEDICINAL CHEMISTRY SECTION NEWSLETTER

This Newsletter is produced semiannually, usually in June and December, by the Secretary of the Medicinal Chemistry Section, Dr. A. I. RACHLIN, with the cooperation of Hoffman-La Roche Inc. It gives details of relevant future meetings from throughout the world and data on the first introduction of new single drugs, together with miscellaneous information of interest to those working in the field of medicinal chemistry. Newsletter No. 11 was issued in June 1975 and No. 12 is scheduled for release in December 1975. A gratis copy may be obtained by writing to the IUPAC Secretariat.

NEW IUPAC PUBLICATIONS FROM BUTTERWORTHS

Manual of Symbols and Terminology for Physicochemical Quantities and Units: 1973 Edition

The IUPAC Commission on Physicochemical Symbols, Terminology, and Units has as its general responsibility to secure clarity and precision, and wider agreement in the use of symbols, by chemists in different countries, among physicists, chemists, and engineers, and by editors of scientific journals. In pursuing these aims, liaison is maintained with other international organizations and in particular with the Commission on Symbols, Units and Nomenclature (SUN Commission) of IUPAP and Technical Committee 12 of ISO.

The text of the 1969 edition of the Manual has been revised by the IUPAC Commission to take account of recent decisions by the Comité International des Poids et Mesures concerning use of the International System of Units, summarized in the document, 'Le Système International d'Unités (SI)', published by the Bureau International des Poids et Mesures in a second edition in 1973 (translations of this document into English have been prepared jointly and published separately by the UK National Physical Laboratory and the US National Bureau of Standards. Section 2.8 of the Manual has been revised in collaboration with IUPAC's Commission on Molecular Structure and Spectroscopy.

viii+42 pages

\$9.00 or £3.00

Ion Exchange Equilibrium Constants

The IUPAC Commission on Equilibrium Data decided at its meeting in Paris in 1965 to make a test compilation of equilibrium constants for ion exchange reactions, in order to consider whether these could be included in the Supplement to *Stability Constants of Metal-Ion Complexes* then being prepared under its sponsorship. The compilation made by Y. MARCUS in 1967 was discussed at the Commission's meeting in Prague in 1967, and it was decided to postpone action. At the meeting in Washington in 1971, it was decided to take up the project again, and Prof. MARCUS was asked to bring the compilation up to date, with the help of G. N. NANCOLLAS.

In a consultation between them, it was decided to keep the previous format, and to prepare an updated compilation. D. G. HOWERY volunteered to help, and provided a great deal of material for the compilation. An early draft was circulated among the Members of the Commission and was approved in principle. That draft has now been completed with further data and brought up to date to the end of 1971.

v+41 pages

\$9.00 or £3.00

Kinetic Parameters of Electrode Reactions of Metallic Compounds

The compilation of kinetic parameters of electrode reactions was started by N. TANAKA and R. TAMAMUSHI, and their first Table appeared in *Electrochimica Acta* 9, 963 (1964). That Table has been used by many electrochemists and kineticists, which encouraged Dr. TAMAMUSHI to continue the work. In 1972 a supplement to the previous Table was prepared in the form of a preprint which covered new data published in the period 1962-1971.

The present Table is a revised and enlarged edition of the previous two Tables, including some additional data published up to the end of 1972. Like its precursors, the new compilation is limited to the electrochemical kinetic parameters of charge transfer processes of metallic compounds; the kinetic data of accompanying processes (e.g., mass transport, preceding and following reactions, etc.) and the kinetic parameters for electrode reactions of nonmetallic and organic substances are excluded. The compilation is not a critical one and, consequently, the parameters given should not be interpreted as recommended values.

For several years the compilation has been undertaken as one of the activities of the IUPAC Commission on Electrochemistry and the work is being continued to cover the ever increasing information available.

xv+176 pages

\$30.00 or £10.00

NEW APPENDICES TO IUPAC INFORMATION BULLETIN

The following *Appendices on Provisional Nomenclature, Symbols, Units, and Standards* were issued in September 1975:

- No. 45 List of Trivial Names and Synonyms (for substances used in analytical chemistry) (Commission on Analytical Nomenclature)
- No. 46 Nomenclature of α -Amino Acids (Commission on Nomenclature of Organic Chemistry and IUPAC-IUB Commission on Biochemical Nomenclature)
- No. 47 Nomenclature of Tocopherols and Related Compounds (IUPAC-IUB Commission on Biochemical Nomenclature)
- No. 48 Nomenclature of Peptide Hormones (IUPAC-IUB Commission on Biochemical Nomenclature)

Gratis copies may be obtained by writing to:

Assistant Secretary (Publications)
IUPAC Secretariat
Bank Court Chambers
2-3 Pound Way
Cowley Centre
Oxford OX4 3YF, UK

Subscribers to the *Information Bulletin* receive all Appendices automatically and free-of-charge on publication. For Appendices issued earlier, see *Information Bulletin* No. 49 (March 1975, p. 131).

Subject to the prior agreement of IUPAC, its provisional nomenclature recommendations may be:

- (a) Republished in other journals.
- (b) Translated into other languages through the National Adhering Organizations of the Union.

CALENDAR OF IUPAC-SPONSORED MEETINGS

1976

June 21-25	International Conference on Colloids and Surfaces (MILTON KERKER, Clarkson College of Technology, Potsdam, New York 13676, USA)	San Juan (Puerto Rico)
June 2-4	II IUPAC Symposium on Photochemical Processes in Polymer Chemistry (Prof. F. C. DE SCHRYVER, Secretary of Organizing Committee, II IUPAC Symposium on Photochemical Processes in Polymer Chemistry, Laboratorium voor Macromoleculaire en Organische Scheikunde, Universiteit te Leuven, Celestijnenlaan 200 F, B-3030 Heverlee, Belgium)	Leuven (Belgium)
June 28 -July 3	V International Fermentation Symposium (V International Fermentation Symposium, Institut für Gärungsgewerbe und Biotechnologie, Seestrasse 13, D-1000 Berlin 65, Federal Republic of Germany)	Berlin (Federal Republic of Germany)
July 5-9	II International Symposium on Polyvinylchloride (Prof. A. GUYOR, Chairman of Organizing Committee, II International Symposium on Polyvinylchloride, LA 199 -Section Cinétique, Chimique, Macromoléculaire, Centre National de la Recherche Scientifique, 39 Boulevard du 11 Novembre 1918, F-69626 Villeurbanne)	Lyon- Villeurbanne (France)
July 6-9	V International Conference on Nonaqueous Solutions (Dr. J. B. GILL, Secretary of Organizing Committee, V International Conference on Nonaqueous Solutions, Department of Inorganic and Structural Chemistry, University of Leeds, Leeds LS2 9JT, UK)	Leeds (UK)
July 6-10	Presymposium on Naturally Occurring Sulfur Compounds (Prof. J. T. WROBEL, Department of Chemistry, University of Warsaw, Pasteura 1, PL 02-093 Warszawa, Poland)	Jablonna (Poland)
July 12-16	V Discussion Conference on Macromolecules: Phases and Interfaces in Macromolecular Systems/XVI Prague Microsymposium on Macromolecules: Advances in Scattering Methods (PMM Secretariat, c/o Institute of Macromolecular Chemistry, Czechoslovak Academy of Sciences, CS-162 06 Praha 616-Petřiny Czechoslovakia)	Prague (Czechoslovakia)
July 12-16	VI International Congress on Catalysis (Dr. J. F. GIBSON, VI International Congress on Catalysis, Chemical Society, Burlington House, Piccadilly, London W1V 0BN, UK)	London (UK)
July 19-22	V International Symposium on Medicinal Chemistry (Dr. J. THUILLIER, Chairman of Organizing Committee, V International Symposium on Medicinal Chemistry, Société de Chimie Thérapeutique, 6-12 Rue Raffet, F-75016 Paris, France)	Paris (France)
July 19-23	VI IUPAC Symposium on Photochemistry (Prof. K. SCHAFFNER, Chairman of Organizing Committee, VI IUPAC Symposium on Photochemistry, Département de Chimie Organique, Université de Genève, 30 Quai Ernest Ansermet, CH-1211 Genève 4, Switzerland)	Aix-en-Provence (France)
August 16-21	VIII International Symposium on Carbohydrate Chemistry (Dr. A. MISAKI, General Secretary, VIII International Symposium on Carbohydrate Chemistry, c/o Kyoto International Conference Hall, Takara-ike, Sakyo-ku, Kyoto 606, Japan)	Kyoto (Japan)

August 23-27	International Symposium on Analytical Chemistry in the Exploration, Mining, and Processing of Materials (Conference Division (IUPAC Symposium), Council for Scientific and Industrial Research, POB 395, Pretoria 0001, Republic of South Africa)	Johannesburg (Republic of South Africa)
August 23-28	X International Symposium on Chemistry of Natural Products (Mr. L. C. SOMERVILLE, Royal Society of New Zealand, 6 Halswell Street, POB 12-249, Wellington, New Zealand)	Dunedin (New Zealand)
August 30 -September 1	Microsymposium on Longterm Properties of Polymers and Polymeric Materials (Prof. B. RÅNBY, Department of Polymer Technology, Royal Institute of Technology, S-100 44 Stockholm 70, Sweden)	Stockholm (Sweden)
August 30 -September 3	VII International Mass Spectrometry Conference (Dr. S. FACCETTI, Chairman of Organizing Committee, VII International Mass Spectrometry Conference, Joint Research Centre, EURATOM, I-21020 Ispra (VA), Italy)	Florence (Italy)
September 6-10	III IUPAC Conference on Physical Organic Chemistry (Prof. G. LAMATY, Laboratoire de Chimie Organique Physique, Université des Sciences et Techniques du Languedoc, Place Eugène Bataillon, F-34060 Montpellier Cedex, France)	Montpellier (France)
September 6-10	XVII International Conference on Coordination Chemistry (Dr. W. FRITSCHÉ, Secretariat of XVII ICC, c/o Gesellschaft Deutscher Chemiker, POB 900440, D-6000 Frankfurt/Main 90, Federal Republic of Germany)	Hamburg (Federal Republic of Germany)
September 7-10	IUPAC-IUFoST Symposium on Advances in Smoking of Foods (Prof. A. RUTKOWSKI, Chairman of Organizing Committee, IUPAC-IUFoST Symposium on Advances in Smoking of Foods, Department of Food Technology, University of Warsaw, Grochowska 272, PL 03-849 Warszawa, Poland)	Warsaw (Poland)
November 9-10	IUPAC Symposium on Techniques for Information Retrieval in Chemistry (Dr. J. F. GIBSON, IUPAC Symposium on Techniques for Information Retrieval in Chemistry, Chemical Society, Burlington House, Piccadilly, London W1V 0BN, UK)	London (UK)
1977		
March 3-5	International Symposium on Clinical Chemistry and Chemical Toxicology of Metals (Trans World Conference Organisers Ltd., 31 Plane Tree Way, Woodstock, Oxford OX7 1PE, UK)	Monte Carlo (Monaco)
May 19-26	VI International Symposium on Magnetic Resonance (Prof. F. H. A. RUMMENS, Department of Chemistry, University of Regina, Regina, Saskatchewan, Canada/ Prof. J. A. WEIL, Department of Chemistry and Chemical Engineering, University of Saskatchewan, Saskatoon, Saskatchewan, Canada)	Banff, Alberta (Canada)
May 22-27	International Symposium of Microchemical Techniques 1977 (Dr. W. MERZ, Chairman of Organizing Committee, International Symposium on Microchemical Techniques, Untersuchungslaboratorium, BASF Aktiengesellschaft, D-6700 Ludwigshafen/Rhein, Federal Republic of Germany)	Davos (Switzerland)
July 17-22	V International Conference on Crystal Growth (R. A. LAUDISE, Joint Chairman of Organizing Committee, ICCG-5, Materials Research Laboratory, Bell Laboratories, 600 Mountain Avenue, Murray Hill, New Jersey 07974, USA)	Cambridge, Massachusetts (USA)

July 17-22	1977 SAC International Symposium on Analytical Chemistry (Dr. G. W. C. MILNER, Chairman of Analytical Division, Chemical Society, 9-10 Savile Row, London W1X 1AF, UK)	Birmingham (UK)
July 18-23	XVIII International Conference on Coordination Chemistry (Prof. P. SENISE, Chairman of Organizing Committee, XVIII International Conference on Coordination Chemistry, Instituto de Química, Universidade de São Paulo, Caixa Postal 20780, São Paulo, Brazil)	São Paulo (Brazil)
September 4-10	26th IUPAC Congress (26th IUPAC Congress, POB 56, Kanda Post Office, Tokyo 101-91, Japan)	Tokyo (Japan)
1978		
July 24-28	IV International Congress of Pesticide Chemistry (IV International Congress of Pesticide Chemistry, POB 182, CH-4013 Basle, Switzerland)	Zürich (Switzerland)

CALENDAR OF NON-IUPAC MEETINGS

1976

February 16-21	International Symposium on Arid Lands Irrigation in Developing Countries (Mr. GAMUL ABDEL SAMIE, Vice-President, Academy of Sciences, Organizing Committee for COWAR Symposium, 102 Kasr el Aini Street, Cairo, Arab Republic of Egypt)	Alexandria (Arab Republic of Egypt)
April 5-9	Annual Chemical Congress of Chemical Society and Royal Institute of Chemistry (Dr. J. F. GIBSON, Chemical Society, Burlington House, Piccadilly, London W1V 0BN, UK)	Glasgow (UK)
May 12-14	9th Congress of International Association for Cereal Chemistry (Dr. H. FUCHS, Secretary General ICC, Schmidgasse 3-7, A-2320 Schwechat, Austria)	Vienna (Austria)
June 1-2	IV Symposium on Radiation Chemistry (Mrs. A. SOMOGYI, Scientific Secretary of Organizing Committee, c/o Hungarian Chemical Society, POB 240, H-1368 Budapest, Hungary)	Keszthely (Hungary)
June 20-26	European Meeting of Chemical Engineering 1976—ACHEMA 1976 (DECHEMA, Postfach 970146, D-6000 Frankfurt/Main 97, Federal Republic of Germany)	Frankfurt Main (Federal Republic of Germany)
June 28 -July 1	Chemical Engineering World Congress (Dr. W. T. KOETSIER and Prof. W. P. M. VAN SWAAIJ, Chemical Engineering World Congress Secretaries, POB 217, Enschede, Netherlands)	Amsterdam (Netherlands)
August 23-27	International Conference on Analysis of Geological Materials (Ing. N. BAJOVÁ, INTERAN '76, House of Technology, SVTS, CS-011 80 Zilina, Czechoslovakia)	Prague (Czechoslovakia)
August 23-27	VII International Congress on Rheology (Prof. J. KUBÁT, Chalmers University of Technology, Fack, S-402 20 Gothenburg 5, Sweden)	Gothenburg (Sweden)

LIST OF ABBREVIATIONS

ACS	American Chemical Society
AOAC	Association of Official Analytical Chemists
CAS	Chemical Abstracts Service
CCPR	FAO-WHO Codex Alimentarius Commission on Pesticide Residues
CEE	Communauté Européenne Economique
CODATA	ICSU Committee on Data for Science and Technology
COMECON	Council of Mutual Economic Assistance of Communist Nations
COWAR	ICSU Committee on Water Research
EPA	US Environmental Protection Agency
EPPO	European Plant Protection Organization
EUSIDIC	European Association of Scientific Information Dissemination Centres
FAO	UN Food and Agriculture Organization
FATIPEC	Fédération d'Associations de Techniciens des Industries des Peinture
FSPT	US Federation of Societies of Paint Technology
IAEA	International Atomic Energy Agency
IAH	International Association of Hydrogeologists
IASH	International Association of Scientific Hydrology
IARC	WHO International Agency for Research on Cancer
IAWPR	International Association on Water Pollution Research
ICCCI	International Coordinating Committee of the Coatings Industry
ICID	International Commission on Irrigation and Drainage
ICOLD	International Commission on Large Dams
ICSU	International Council of Scientific Unions
ICSU AB	ICSU Abstracting Board
ICTA	International Confederation for Thermal Analysis
ISO	International Organization for Standardization
ISO/TC	ISO Technical Committee
IFCC	International Federation of Clinical Chemistry
IOCG	International Organization for Crystal Growth
ISDS	International Serials Data System
ISSS	International Society of Soil Science
IUB	International Union of Biochemistry
IUBS	International Union of Biological Sciences
IUCr	International Union of Crystallography
IUFoST	International Union of Food Science and Technology
IUPHAR	International Union of Pharmacology
IUPAP	International Union of Pure and Applied Physics
JMPR	Joint Meeting of FAO-WHO Experts on Pesticide Residues
MAB	Man and the Biosphere Programme
OCCA	UK Oil and Colour Chemists' Association
OECD	Organization for Economic Cooperation and Development
SCOPE	ICSU Scientific Committee on Problems of the Environment
SLF	Federation of Scandinavian Paint and Varnish Technicians
UN	United Nations
UNESCO	UN Educational, Scientific, and Cultural Organization
UNEP	UN Environment Programme
UNISIST	UNESCO-ICSU Programme on International Science Information System
WHO	UN World Health Organization
WMO	World Meteorological Organization
WPSPF	IUPAC Macromolecular Division Working Party on Supported Polymer Films

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